

Triphenylmethane

Other names:	1,1',1''-Methylidynetris[benzene] 1,1',1''-methylidynetrisbenzene Benzene,1,1',1''-methylidynetris- benzene, 1,1',1''-methylidynetris- methane, triphenyl- tritane
Inchi:	InChI=1S/C19H16/c1-4-10-16(11-5-1)19(17-12-6-2-7-13-17)18-14-8-3-9-15-18/h1-15,19H
InchiKey:	AAQKTZKLRYKHR-UHFFFAOYSA-N
Formula:	C19H16
SMILES:	c1ccc(C(c2ccccc2)c2ccccc2)cc1
Mol. weight [g/mol]:	244.33
CAS:	519-73-3

Physical Properties

Property code	Value	Unit	Source
gf	443.89	kJ/mol	Joback Method
hf	276.10 ± 5.00	kJ/mol	NIST Webbook
hfus	23.57	kJ/mol	Joback Method
hsub	109.10 ± 0.60	kJ/mol	NIST Webbook
hsub	100.70	kJ/mol	NIST Webbook
hsub	112.00	kJ/mol	NIST Webbook
hsub	108.40 ± 2.80	kJ/mol	NIST Webbook
hsub	105.00 ± 0.80	kJ/mol	NIST Webbook
hvap	93.20 ± 2.20	kJ/mol	NIST Webbook
hvap	94.60	kJ/mol	NIST Webbook
hvap	95.00	kJ/mol	NIST Webbook
ie	8.40 ± 0.05	eV	NIST Webbook
ie	8.34 ± 0.03	eV	NIST Webbook
ie	8.34 ± 0.04	eV	NIST Webbook
log10ws	-5.25		Crippen Method
logp	4.867		Crippen Method
mcvol	207.290	ml/mol	McGowan Method
pc	2400.57	kPa	Joback Method
rinpol	327.80		NIST Webbook
rinpol	1997.00		NIST Webbook
rinpol	1982.00		NIST Webbook
rinpol	327.80		NIST Webbook

rinpol	1982.00		NIST Webbook
rinpol	1978.00		NIST Webbook
rinpol	1997.00		NIST Webbook
sg	541.00	J/mol×K	NIST Webbook
tb	632.00 ± 1.00	K	NIST Webbook
tb	632.00 ± 6.00	K	NIST Webbook
tb	449.00 ± 2.00	K	NIST Webbook
tc	982.16	K	Joback Method
tf	362.00 ± 7.00	K	NIST Webbook
tf	364.40 ± 3.00	K	NIST Webbook
tf	365.70 ± 3.00	K	NIST Webbook
tf	367.80 ± 3.00	K	NIST Webbook
tf	366.40 ± 1.00	K	NIST Webbook
tf	365.00 ± 6.00	K	NIST Webbook
tf	361.00 ± 6.00	K	NIST Webbook
tf	365.00 ± 0.10	K	NIST Webbook
tf	363.00 ± 4.00	K	NIST Webbook
tf	365.00 ± 4.00	K	NIST Webbook
tf	365.70 ± 1.50	K	NIST Webbook
tf	365.50 ± 1.00	K	NIST Webbook
tf	365.20 ± 1.00	K	NIST Webbook
tf	365.20 ± 0.50	K	NIST Webbook
tf	365.00 ± 3.00	K	NIST Webbook
tf	366.40 ± 1.50	K	NIST Webbook
tf	365.60 ± 0.20	K	NIST Webbook
tf	363.00 ± 2.00	K	NIST Webbook
tf	365.00 ± 4.00	K	NIST Webbook
tf	365.30 ± 0.20	K	NIST Webbook
tf	366.00 ± 2.00	K	NIST Webbook
tf	365.30 ± 1.00	K	NIST Webbook
tf	366.85 ± 0.30	K	NIST Webbook
tf	366.25 ± 0.20	K	NIST Webbook
tf	365.50 ± 0.60	K	NIST Webbook
tf	365.99 ± 0.50	K	NIST Webbook
vc	0.769	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	586.50	J/mol×K	803.20	Joback Method
cpg	550.53	J/mol×K	713.72	Joback Method

cpg	569.41	J/mol×K	758.46	Joback Method
cpg	640.21	J/mol×K	982.16	Joback Method
cpg	601.97	J/mol×K	847.94	Joback Method
cpg	615.98	J/mol×K	892.68	Joback Method
cpg	628.67	J/mol×K	937.42	Joback Method
dvisc	0.0002819	Pa×s	540.94	Joback Method
dvisc	0.0004615	Pa×s	483.34	Joback Method
dvisc	0.0008632	Pa×s	425.75	Joback Method
dvisc	0.0001036	Pa×s	713.72	Joback Method
dvisc	0.0001364	Pa×s	656.12	Joback Method
dvisc	0.0001893	Pa×s	598.53	Joback Method
dvisc	0.0019643	Pa×s	368.15	Joback Method
hfust	21.97	kJ/mol	365.30	NIST Webbook
hfust	20.70	kJ/mol	367.20	NIST Webbook
hfust	21.97	kJ/mol	365.30	NIST Webbook
hfust	18.20	kJ/mol	365.50	NIST Webbook
hfust	21.98	kJ/mol	365.30	NIST Webbook
hfust	20.92	kJ/mol	365.60	NIST Webbook
hsubt	113.90	kJ/mol	353.00	NIST Webbook
hsubt	100.00 ± 0.40	kJ/mol	337.00	NIST Webbook
hsubt	106.70 ± 0.60	kJ/mol	338.00	NIST Webbook
hsubt	100.10 ± 0.59	kJ/mol	367.00	NIST Webbook
hsubt	106.80	kJ/mol	330.50	NIST Webbook
hvapt	82.00	kJ/mol	402.50	NIST Webbook
hvapt	58.60	kJ/mol	577.50	NIST Webbook
pvap	0.19	kPa	470.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.92	kPa	510.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.64	kPa	500.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	0.44	kPa	490.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.29	kPa	480.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.12	kPa	460.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.07	kPa	450.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.04	kPa	440.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.03	kPa	430.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.01	kPa	420.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	7.52e-03	kPa	410.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	3.87e-03	kPa	400.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.90e-03	kPa	390.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	8.85e-04	kPa	380.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	3.91e-04	kPa	370.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.63e-04	kPa	360.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	6.36e-05	kPa	350.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	2.31e-05	kPa	340.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.39e-06	kPa	320.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	6.70e-07	kPa	310.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.69e-07	kPa	300.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.30e-07	kPa	298.15	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	7.76e-06	kPa	330.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
sfust	57.20	J/mol×K	365.60	NIST Webbook
sfust	49.80	J/mol×K	365.50	NIST Webbook
sfust	60.20	J/mol×K	365.30	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	631.70	K	101.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C519733&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Hypothetical Thermodynamic Properties. Subcooled Vaporization	https://www.doi.org/10.1021/je800300x
Joback Method	https://en.wikipedia.org/wiki/Joback_method
Joback Method Vapor Pressures of Polyaromatic Hydrocarbons:	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
sg:	Molar entropy at standard conditions
tb:	Normal Boiling Point Temperature

tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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