

Triphenylene, 1,2,3,4,5,6,7,8,9,10,11,12-dodecahydro-

Other names:	Dodecahydrotriphenylene Tritetralin 1,2,3,4,5,6,7,8,9,10,11,12-Dodecahydrotriphenylene Dodecahydrotri-o-phenylene
Inchi:	InChI=1S/C18H24/c1-2-8-14-13(7-1)15-9-3-4-11-17(15)18-12-6-5-10-16(14)18/h1-12H2
InchiKey:	ODHYDPYRIQKHCI-UHFFFAOYSA-N
Formula:	C18H24
SMILES:	C1CCc2c(c3c(c4c2CCCC4)CCCC3)C1
Mol. weight [g/mol]:	240.38
CAS:	1610-39-5

Physical Properties

Property code	Value	Unit	Source
chs	-10319.20 ± 1.40	kJ/mol	NIST Webbook
gf	334.02	kJ/mol	Joback Method
hf	25.27	kJ/mol	Joback Method
hfs	-193.90 ± 1.70	kJ/mol	NIST Webbook
hfus	19.36	kJ/mol	Joback Method
hvap	62.43	kJ/mol	Joback Method
ie	8.60 ± 0.03	eV	NIST Webbook
ie	7.70 ± 0.05	eV	NIST Webbook
log10ws	-5.97		Crippen Method
logp	4.323		Crippen Method
mcvol	208.140	ml/mol	McGowan Method
pc	2212.45	kPa	Joback Method
rinpol	386.36		NIST Webbook
tb	709.86	K	Joback Method
tc	958.95	K	Joback Method
tf	509.15 ± 1.00	K	NIST Webbook
vc	0.785	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	614.13	J/molxK	709.86	Joback Method
cpg	635.71	J/molxK	751.38	Joback Method
cpg	655.76	J/molxK	792.89	Joback Method
cpg	674.45	J/molxK	834.41	Joback Method
cpg	691.94	J/molxK	875.92	Joback Method
cpg	708.41	J/molxK	917.44	Joback Method
cpg	724.04	J/molxK	958.95	Joback Method
dvisc	0.0021848	Paxs	437.62	Joback Method
dvisc	0.0015437	Paxs	482.99	Joback Method
dvisc	0.0011577	Paxs	528.37	Joback Method
dvisc	0.0009087	Paxs	573.74	Joback Method
dvisc	0.0007390	Paxs	619.11	Joback Method
dvisc	0.0006182	Paxs	664.49	Joback Method
dvisc	0.0005291	Paxs	709.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1610395&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure

rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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