

Triphenylethylene

Other names:	1,1,2-Triphenylethylene 1,2,2-Triphenylethylene Benzilidenediphenylmethane Ethylene, triphenyl- Triphenylethene
Inchi:	InChI=1S/C20H16/c1-4-10-17(11-5-1)16-20(18-12-6-2-7-13-18)19-14-8-3-9-15-19/h1-16
InchiKey:	MKYQPGPNVYRMHI-UHFFFAOYSA-N
Formula:	C20H16
SMILES:	C(=C(c1ccccc1)c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	256.35
CAS:	58-72-0

Physical Properties

Property code	Value	Unit	Source
chs	-10390.20 ± 1.70	kJ/mol	NIST Webbook
chs	-10503.00	kJ/mol	NIST Webbook
hf	377.76	kJ/mol	Cheméo Relay (1.0)
hfus	28.57	kJ/mol	Joback Method
hsub	112.20 ± 1.90	kJ/mol	NIST Webbook
hvap	91.80 ± 0.90	kJ/mol	NIST Webbook
ie	7.61	eV	Cheméo Relay (1.0)
logp	5.275		Crippen Method
mcvol	217.080	ml/mol	McGowan Method
tb	651.73	K	Cheméo Relay (1.0)
tf	337.00 ± 4.00	K	NIST Webbook
tf	339.00 ± 0.70	K	NIST Webbook
tf	342.40 ± 2.00	K	NIST Webbook
tf	339.00 ± 4.00	K	NIST Webbook
tf	342.00 ± 4.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	629.69	J/mol×K	877.06	Joback Method

cpg	579.64	J/mol×K	741.08	Joback Method
cpg	597.95	J/mol×K	786.41	Joback Method
cpg	614.57	J/mol×K	831.73	Joback Method
cpg	643.51	J/mol×K	922.39	Joback Method
cpg	656.23	J/mol×K	967.71	Joback Method
cpg	668.04	J/mol×K	1013.04	Joback Method
cps	309.20	J/mol×K	298.50	NIST Webbook
hfust	20.58	kJ/mol	339.90	NIST Webbook
hfust	20.35	kJ/mol	341.00	NIST Webbook
hsubt	110.10 ± 1.90	kJ/mol	331.00	NIST Webbook
hvapt	88.00 ± 0.90	kJ/mol	361.50	NIST Webbook
hvapt	89.70	kJ/mol	398.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	493.70	K	1.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	2.07265e+01
Coeff. B	-8.22374e+03
Coeff. C	-9.72000e+01
Temperature range (K), min.	499.56
Temperature range (K), max.	630.69

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	1.53479e+02
Coeff. B	-1.70969e+04
Coeff. C	-1.93870e+01
Coeff. D	6.20138e-06
Temperature range (K), min.	342.15

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C58720&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB Vapor Pressure Data:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=814
Crippen Method:	https://www.chemed.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
KDB:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=814
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0, beta):	

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
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
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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