1,1,2-Triphenylethane

Other names: Ethane, 1,1,2-triphenyl-
1,1,2-Triphenylethane
Inchi: InChI=1S/C20H18/c1-4-10-17(11-5-1)16-20(18-12-6-2-7-13-18)19-14-8-3-9-15-19/h1-15,
InchiKey: KIIBETRYVBIAOO-UHFFFAOYSA-N
Formula: C20H18
SMILES: c1ccc(CC(c2ccccc2)c2ccccc2)cc1
Mol. weight [g/mol]: 258.36

Physical Properties

Property code	Value	Unit	Source
af	0.4897		Cheméo Relay (1.0)
chs	-10572.90 ± 2.00	kJ/mol	NIST Webbook
gf	452.31	kJ/mol	Joback Method
hf	262.78	kJ/mol	Cheméo Relay (1.0)
hfus	26.16	kJ/mol	Joback Method
hsub	92.20 ± 0.50	kJ/mol	NIST Webbook
hvap	95.64	kJ/mol	Cheméo Relay (1.0)
ie	8.40	eV	Cheméo Relay (1.0)
log10ws	-6.16		Cheméo Relay (1.0)
logp	5.061		Crippen Method
mcvol	221.380	ml/mol	McGowan Method
pc	2189.73	kPa	Joback Method
tb	624.12	K	Cheméo Relay (1.0)
tc	909.24	K	Cheméo Relay (1.0)
tf	321.15 ± 1.00	K	NIST Webbook
tf	327.30 ± 0.30	K	NIST Webbook
tf	328.00 ± 4.00	K	NIST Webbook
tf	327.70 ± 2.00	K	NIST Webbook
tf	327.80 ± 0.60	K	NIST Webbook
tf	328.40 ± 2.00	K	NIST Webbook
tf	324.00 ± 3.00	K	NIST Webbook
tf	327.00 ± 4.00	K	NIST Webbook
tf	329.00 ± 2.00	K	NIST Webbook
tf	329.30 ± 3.00	K	NIST Webbook
vc	0.809	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.87	J/mol×K	954.88	Joback Method
cpg	695.73	J/mol×K	998.54	Joback Method
cpg	670.88	J/mol×K	911.23	Joback Method
cpg	604.73	J/mol×K	736.60	Joback Method
cpg	623.70	J/mol×K	780.26	Joback Method
cpg	640.95	J/mol×K	823.91	Joback Method
cpg	656.63	J/mol×K	867.57	Joback Method
cps	319.70	J/mol×K	298.50	NIST Webbook
dvisc	0.0018214	Pa×s	379.42	Joback Method
dvisc	0.0007915	Pa×s	438.95	Joback Method
dvisc	0.0004197	Pa×s	498.48	Joback Method
dvisc	0.0002548	Pa×s	558.01	Joback Method
dvisc	0.0001703	Pa×s	617.54	Joback Method
dvisc	0.0001222	Pa×s	677.07	Joback Method
dvisc	0.0000925	Pa×s	736.60	Joback Method
hfust	24.39	kJ/mol	328.20	NIST Webbook
hsubt	89.00 ± 0.50	kJ/mol	351.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1520429&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

af: Acentric Factor

chs: Standard solid enthalpy of combustion

cpg: Ideal gas heat capacity

cps:	Solid phase 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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume