Triphenylcyclopropene

Other names:	1,2,3-Triphenylcyclopropene
	Benzene, 1,1',1''-(1-cyclopropene-1,2,3-triyl)tris-
	Cyclopropene, 1,2,3-triphenyl-
	1,1',1''-(1-cyclopropene-1,2,3-triyl)trisbenzene
Inchi:	InChI=1S/C21H16/c1-4-10-16(11-5-1)19-20(17-12-6-2-7-13-17)21(19)18-14-8-3-9-15-18/
InchiKey:	UFTDGVXRVMJEDI-UHFFFAOYSA-N
Formula:	C21H16
SMILES:	c1ccc(C2=C(c3ccccc3)C2c2ccccc2)cc1
Mol. weight [g/mol]:	268.35
CAS:	16510-49-9

Physical Properties

Property code	Value	Unit	Source
gf	534.62	kJ/mol	Joback Method
hf	340.46	kJ/mol	Joback Method
hfus	30.85	kJ/mol	Joback Method
hvap	70.70	kJ/mol	Joback Method
log10ws	-5.97		Crippen Method
logp	5.395		Crippen Method
mcvol	220.310	ml/mol	McGowan Method
pc	2256.81	kPa	Joback Method
tb	775.78	K	Joback Method
tc	1047.30	K	Joback Method
tf	449.43	K	Joback Method
vc	0.831	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	615.04	J/mol×K	775.78	Joback Method
cpg	690.08	J/mol×K	1002.05	Joback Method
cpg	677.34	J/mol×K	956.80	Joback Method
cpg	663.67	J/mol×K	911.54	Joback Method
cpg	648.87	J/mol×K	866.29	Joback Method

cpg	632.73	J/mol×K	821.03	Joback Method
cpg	702.10	J/mol×K	1047.30	Joback Method
dvisc	0.0002828	Pa×s	775.78	Joback Method
dvisc	0.0003327	Pa×s	721.39	Joback Method
dvisc	0.0004020	Pa×s	667.00	Joback Method
dvisc	0.0005024	Pa×s	612.61	Joback Method
dvisc	0.0006556	Pa×s	558.21	Joback Method
dvisc	0.0009063	Pa×s	503.82	Joback Method
dvisc	0.0013548	Pa×s	449.43	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16510499&Units=SI

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
hvap: Enthalpy of vaporization at standard conditions
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

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