

Triphenylmethane, 4,4',4''-trichloro

Inchi: InChI=1S/C19H13Cl3/c20-16-7-1-13(2-8-16)19(14-3-9-17(21)10-4-14)15-5-11-18(22)12-6
InchiKey: WAGIESWOTQOLJS-UHFFFAOYSA-N
Formula: C19H13Cl3
SMILES: Clc1ccc(C(c2ccc(Cl)cc2)c2ccc(Cl)cc2)cc1
Mol. weight [g/mol]: 347.67

Physical Properties

Property code	Value	Unit	Source
gf	379.21	kJ/mol	Joback Method
hf	187.19	kJ/mol	Joback Method
hfus	34.99	kJ/mol	Joback Method
hvap	79.47	kJ/mol	Joback Method
log10ws	-7.31		Crippen Method
logp	6.827		Crippen Method
mcvol	244.010	ml/mol	McGowan Method
pc	2071.76	kPa	Joback Method
rinpol	421.20		NIST Webbook
rinpol	421.20		NIST Webbook
tb	840.95	K	Joback Method
tc	1115.16	K	Joback Method
tf	495.47	K	Joback Method
vc	0.916	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.86	J/mol×K	840.95	Joback Method
cpg	632.31	J/mol×K	886.65	Joback Method
cpg	644.43	J/mol×K	932.35	Joback Method
cpg	655.35	J/mol×K	978.06	Joback Method
cpg	665.21	J/mol×K	1023.76	Joback Method
cpg	674.16	J/mol×K	1069.46	Joback Method
cpg	682.33	J/mol×K	1115.16	Joback Method
dvisc	0.0006656	Pa×s	495.47	Joback Method

dvisc	0.0003856	Pa×s	553.05	Joback Method
dvisc	0.0002476	Pa×s	610.63	Joback Method
dvisc	0.0001716	Pa×s	668.21	Joback Method
dvisc	0.0001261	Pa×s	725.79	Joback Method
dvisc	0.0000969	Pa×s	783.37	Joback Method
dvisc	0.0000772	Pa×s	840.95	Joback Method

Sources

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=R396288&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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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