

Triphenylmethane, 2,4-dichloro

Inchi:	InChI=1S/C19H14Cl2/c20-16-11-12-17(18(21)13-16)19(14-7-3-1-4-8-14)15-9-5-2-6-10-1
InchiKey:	SYXAFMYOBOTRHM-UHFFFAOYSA-N
Formula:	C19H14Cl2
SMILES:	Clc1ccc(C(c2ccccc2)c2ccccc2)c(Cl)c1
Mol. weight [g/mol]:	313.22

Physical Properties

Property code	Value	Unit	Source
gf	400.77	kJ/mol	Joback Method
hf	214.40	kJ/mol	Joback Method
hfus	31.18	kJ/mol	Joback Method
hvap	74.42	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	6.174		Crippen Method
mvol	231.770	ml/mol	McGowan Method
pc	2173.43	kPa	Joback Method
rinpol	375.10		NIST Webbook
rinpol	375.10		NIST Webbook
tb	798.54	K	Joback Method
tc	1071.12	K	Joback Method
tf	453.03	K	Joback Method
vc	0.868	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.30	J/molxK	798.54	Joback Method
cpg	660.56	J/molxK	1025.69	Joback Method
cpg	650.48	J/molxK	980.26	Joback Method
cpg	639.36	J/molxK	934.83	Joback Method
cpg	627.05	J/molxK	889.40	Joback Method
cpg	613.41	J/molxK	843.97	Joback Method
cpg	669.76	J/molxK	1071.12	Joback Method
dvisc	0.0000862	Paxs	798.54	Joback Method

dvisc	0.0001097	Paxs	740.95	Joback Method
dvisc	0.0001453	Paxs	683.37	Joback Method
dvisc	0.0002029	Paxs	625.78	Joback Method
dvisc	0.0003031	Paxs	568.20	Joback Method
dvisc	0.0004956	Paxs	510.62	Joback Method
dvisc	0.0009183	Paxs	453.03	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R396248&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
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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