

1,1-bis-(4-Methylphenyl)-2,2-dichloroethylene

Inchi:	InChI=1S/C16H14Cl2/c1-11-3-7-13(8-4-11)15(16(17)18)14-9-5-12(2)6-10-14/h3-10H,1-2
InchiKey:	MSUWJPYRBHVMHQ-UHFFFAOYSA-N
Formula:	C16H14Cl2
SMILES:	<chem>Cc1ccc(C(=C(Cl)Cl)c2ccc(C)cc2)cc1</chem>
Mol. weight [g/mol]:	277.19

Physical Properties

Property code	Value	Unit	Source
gf	328.66	kJ/mol	Joback Method
hf	142.71	kJ/mol	Joback Method
hfus	30.48	kJ/mol	Joback Method
hvap	65.97	kJ/mol	Joback Method
log10ws	-6.26		Crippen Method
logp	5.498		Crippen Method
mvol	208.960	ml/mol	McGowan Method
pc	2195.89	kPa	Joback Method
rinpol	1974.00		NIST Webbook
rinpol	1974.00		NIST Webbook
tb	707.58	K	Joback Method
tc	963.51	K	Joback Method
tf	374.80	K	Joback Method
vc	0.795	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.05	J/mol×K	707.58	Joback Method
cpg	518.41	J/mol×K	750.23	Joback Method
cpg	532.52	J/mol×K	792.89	Joback Method
cpg	545.50	J/mol×K	835.54	Joback Method
cpg	557.46	J/mol×K	878.20	Joback Method
cpg	568.53	J/mol×K	920.85	Joback Method
cpg	578.81	J/mol×K	963.51	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=R68530&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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