

Diphenylmethane, 2,4,4'-trichloro

Inchi:	InChI=1S/C13H9Cl3/c14-11-4-1-9(2-5-11)7-10-3-6-12(15)8-13(10)16/h1-6,8H,7H2
InchiKey:	WZXNQNDMDJGWIZ-UHFFFAOYSA-N
Formula:	C13H9Cl3
SMILES:	Clc1ccc(Cc2ccc(Cl)cc2Cl)cc1
Mol. weight [g/mol]:	271.57

Physical Properties

Property code	Value	Unit	Source
gf	218.72	kJ/mol	Joback Method
hf	79.78	kJ/mol	Joback Method
hfus	28.93	kJ/mol	Joback Method
hvap	64.22	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	5.238		Crippen Method
mcvol	183.230	ml/mol	McGowan Method
pc	2603.08	kPa	Joback Method
rinpol	333.30		NIST Webbook
tb	677.43	K	Joback Method
tc	934.55	K	Joback Method
tf	416.43	K	Joback Method
vc	0.695	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.62	J/molxK	677.43	Joback Method
cpg	410.10	J/molxK	720.28	Joback Method
cpg	421.52	J/molxK	763.14	Joback Method
cpg	431.95	J/molxK	805.99	Joback Method
cpg	441.46	J/molxK	848.84	Joback Method
cpg	450.11	J/molxK	891.69	Joback Method
cpg	457.98	J/molxK	934.55	Joback Method
dvisc	0.0010257	Paxs	416.43	Joback Method
dvisc	0.0006570	Paxs	459.93	Joback Method

dvisc	0.0004545	Paxs	503.43	Joback Method
dvisc	0.0003334	Paxs	546.93	Joback Method
dvisc	0.0002559	Paxs	590.43	Joback Method
dvisc	0.0002038	Paxs	633.93	Joback Method
dvisc	0.0001671	Paxs	677.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R396184&Units=SI
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

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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