

Dichloromethylene bis-(2,4,5-trichlorobenzene)

Inchi:	InChI=1S/C13H4Cl8/c14-7-3-11(18)9(16)1-5(7)13(20,21)6-2-10(17)12(19)4-8(6)15/h1-4H
InchiKey:	NGVUNNHEOBNOAB-UHFFFAOYSA-N
Formula:	C13H4Cl8
SMILES:	Clc1cc(Cl)c(C(Cl)(Cl)c2cc(Cl)c(Cl)cc2Cl)cc1Cl
Mol. weight [g/mol]:	443.80
CAS:	93186-50-6

Physical Properties

Property code	Value	Unit	Source
gf	133.02	kJ/mol	Joback Method
hf	-42.08	kJ/mol	Joback Method
hfus	41.34	kJ/mol	Joback Method
hvap	86.84	kJ/mol	Joback Method
log10ws	-8.65		Crippen Method
logp	8.286		Crippen Method
mcvol	244.430	ml/mol	McGowan Method
pc	2121.68	kPa	Joback Method
tb	876.29	K	Joback Method
tc	1157.62	K	Joback Method
tf	606.01	K	Joback Method
vc	0.928	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.17	J/molxK	876.29	Joback Method
cpg	513.87	J/molxK	1110.73	Joback Method
cpg	509.23	J/molxK	1063.84	Joback Method
cpg	504.25	J/molxK	1016.95	Joback Method
cpg	498.83	J/molxK	970.07	Joback Method
cpg	492.84	J/molxK	923.18	Joback Method
cpg	518.30	J/molxK	1157.62	Joback Method
dvisc	0.0000742	Paxs	876.29	Joback Method
dvisc	0.0000888	Paxs	831.24	Joback Method

dvisc	0.0001085	Paxs	786.20	Joback Method
dvisc	0.0001358	Paxs	741.15	Joback Method
dvisc	0.0001750	Paxs	696.10	Joback Method
dvisc	0.0002336	Paxs	651.06	Joback Method
dvisc	0.0003255	Paxs	606.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C93186506&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
mccvol:	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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