

PCB 201

Inchi:	InChI=1S/C12H2Cl8/c13-4-1-3(8(16)12(20)11(4)19)7-9(17)5(14)2-6(15)10(7)18/h1-2H
InchiKey:	HJBYDWKNARZTMJ-UHFFFAOYSA-N
Formula:	C12H2Cl8
SMILES:	Clc1cc(-c2c(Cl)c(Cl)cc(Cl)c2Cl)c(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	429.77

Physical Properties

Property code	Value	Unit	Source
gf	102.50	kJ/mol	Joback Method
hf	-35.63	kJ/mol	Joback Method
hfus	45.38	kJ/mol	Joback Method
hvap	87.23	kJ/mol	Joback Method
log10ws	-9.55		Crippen Method
logp	8.581		Crippen Method
mcvol	230.340	ml/mol	McGowan Method
pc	2216.62	kPa	Joback Method
rinqol	2502.00		NIST Webbook
tb	866.60	K	Joback Method
tc	1140.81	K	Joback Method
tf	617.36	K	Joback Method
vc	0.883	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.83	J/molxK	866.60	Joback Method
cpg	433.76	J/molxK	912.30	Joback Method
cpg	438.99	J/molxK	958.00	Joback Method
cpg	443.56	J/molxK	1003.70	Joback Method
cpg	447.49	J/molxK	1049.40	Joback Method
cpg	450.83	J/molxK	1095.11	Joback Method
cpg	453.59	J/molxK	1140.81	Joback Method
dvisc	0.0003571	Paxs	617.36	Joback Method
dvisc	0.0002775	Paxs	658.90	Joback Method

dvisc	0.0002223	Paxs	700.44	Joback Method
dvisc	0.0001825	Paxs	741.98	Joback Method
dvisc	0.0001530	Paxs	783.52	Joback Method
dvisc	0.0001305	Paxs	825.06	Joback Method
dvisc	0.0001131	Paxs	866.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R596993&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
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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