

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)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
rinpol	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	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0002223	Pa×s	700.44	Joback Method
dvisc	0.0001825	Pa×s	741.98	Joback Method
dvisc	0.0001530	Pa×s	783.52	Joback Method
dvisc	0.0001305	Pa×s	825.06	Joback Method
dvisc	0.0001131	Pa×s	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/ci990307l
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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