

2,2-Dichloropropionic acid, pentachlorophenyl ester

Inchi:	InChI=1S/C9H3Cl7O2/c1-9(15,16)8(17)18-7-5(13)3(11)2(10)4(12)6(7)14/h1H3
InchiKey:	VAOPRNWCLHADEN-UHFFFAOYSA-N
Formula:	C9H3Cl7O2
SMILES:	CC(Cl)(Cl)C(=O)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	391.29
CAS:	116402-62-1

Physical Properties

Property code	Value	Unit	Source
gf	-225.43	kJ/mol	Joback Method
hf	-413.64	kJ/mol	Joback Method
hfus	35.91	kJ/mol	Joback Method
hvap	79.77	kJ/mol	Joback Method
log10ws	-6.54		Crippen Method
logp	6.053		Crippen Method
mcvol	207.030	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
tb	791.97	K	Joback Method
tc	1048.27	K	Joback Method
tf	564.23	K	Joback Method
vc	0.787	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.38	J/molxK	791.97	Joback Method
cpg	400.17	J/molxK	834.69	Joback Method
cpg	405.32	J/molxK	877.40	Joback Method
cpg	409.86	J/molxK	920.12	Joback Method
cpg	413.81	J/molxK	962.84	Joback Method
cpg	417.21	J/molxK	1005.55	Joback Method
cpg	420.10	J/molxK	1048.27	Joback Method
dvisc	0.0004329	Paxs	564.23	Joback Method
dvisc	0.0003187	Paxs	602.19	Joback Method

dvisc	0.0002432	Paxs	640.14	Joback Method
dvisc	0.0001914	Paxs	678.10	Joback Method
dvisc	0.0001544	Paxs	716.06	Joback Method
dvisc	0.0001273	Paxs	754.01	Joback Method
dvisc	0.0001070	Paxs	791.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402621&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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