

Bis(2,4-dichlorophenoxy)acetic acid

Inchi:	InChI=1S/C14H8Cl4O4/c15-7-1-3-11(9(17)5-7)21-14(13(19)20)22-12-4-2-8(16)6-10(12)1
InchiKey:	CPLNQESJGPCJSC-UHFFFAOYSA-N
Formula:	C14H8Cl4O4
SMILES:	O=C(O)C(Oc1ccc(Cl)cc1Cl)Oc1ccc(Cl)cc1Cl
Mol. weight [g/mol]:	382.02
CAS:	100541-30-8

Physical Properties

Property code	Value	Unit	Source
gf	-272.60	kJ/mol	Joback Method
hf	-502.60	kJ/mol	Joback Method
hfus	39.87	kJ/mol	Joback Method
hvap	99.35	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	5.169		Crippen Method
mcvol	228.740	ml/mol	McGowan Method
pc	2553.34	kPa	Joback Method
tb	933.17	K	Joback Method
tc	1171.97	K	Joback Method
tf	610.35	K	Joback Method
vc	0.855	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	560.10	J/molxK	933.17	Joback Method
cpg	583.67	J/molxK	1132.17	Joback Method
cpg	580.86	J/molxK	1092.37	Joback Method
cpg	577.11	J/molxK	1052.57	Joback Method
cpg	572.41	J/molxK	1012.77	Joback Method
cpg	566.75	J/molxK	972.97	Joback Method
cpg	585.55	J/molxK	1171.97	Joback Method
dvisc	0.0000101	Paxs	933.17	Joback Method
dvisc	0.0000135	Paxs	879.37	Joback Method

dvisc	0.0000187	Paxs	825.56	Joback Method
dvisc	0.0000272	Paxs	771.76	Joback Method
dvisc	0.0000418	Paxs	717.96	Joback Method
dvisc	0.0000688	Paxs	664.15	Joback Method
dvisc	0.0001238	Paxs	610.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100541308&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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