

2-Hydroxy-1-methylpropyl (2,4-dichlorophenoxy)acetate

Inchi:	InChI=1S/C12H14Cl2O4/c1-7(15)8(2)18-12(16)6-17-11-4-3-9(13)5-10(11)14/h3-5,7-8,15
InchiKey:	VXSLRAHUUHDTDM-UHFFFAOYSA-N
Formula:	C12H14Cl2O4
SMILES:	CC(O)C(C)OC(=O)COc1ccc(Cl)cc1Cl
Mol. weight [g/mol]:	293.14
CAS:	116436-38-5

Physical Properties

Property code	Value	Unit	Source
gf	-361.17	kJ/mol	Joback Method
hf	-648.71	kJ/mol	Joback Method
hfus	29.51	kJ/mol	Joback Method
hvap	82.14	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	2.685		Crippen Method
mcvol	199.840	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method
tb	775.47	K	Joback Method
tc	983.54	K	Joback Method
tf	461.51	K	Joback Method
vc	0.747	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.53	J/molxK	775.47	Joback Method
cpg	532.08	J/molxK	810.15	Joback Method
cpg	541.86	J/molxK	844.83	Joback Method
cpg	550.86	J/molxK	879.51	Joback Method
cpg	559.08	J/molxK	914.18	Joback Method
cpg	566.53	J/molxK	948.86	Joback Method
cpg	573.22	J/molxK	983.54	Joback Method
dvisc	0.0006788	Paxs	461.51	Joback Method
dvisc	0.0002808	Paxs	513.84	Joback Method

dvisc	0.0001368	Paxs	566.16	Joback Method
dvisc	0.0000752	Paxs	618.49	Joback Method
dvisc	0.0000454	Paxs	670.82	Joback Method
dvisc	0.0000295	Paxs	723.14	Joback Method
dvisc	0.0000203	Paxs	775.47	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116436385&Units=SI

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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