

6-Methylheptyl (2,4-dichlorophenoxy)acetate

Inchi:	InChI=1S/C16H22Cl2O3/c1-12(2)6-4-3-5-9-20-16(19)11-21-15-8-7-13(17)10-14(15)18/h
InchiKey:	BBPLSOGERZQYQC-UHFFFAOYSA-N
Formula:	C16H22Cl2O3
SMILES:	CC(C)CCCCOC(=O)COc1ccc(Cl)cc1Cl
Mol. weight [g/mol]:	333.25
CAS:	3035-67-4

Physical Properties

Property code	Value	Unit	Source
gf	-188.23	kJ/mol	Joback Method
hf	-573.76	kJ/mol	Joback Method
hfus	39.30	kJ/mol	Joback Method
hvap	74.76	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	5.132		Crippen Method
mvol	250.330	ml/mol	McGowan Method
pc	1612.88	kPa	Joback Method
tb	775.25	K	Joback Method
tc	981.60	K	Joback Method
tf	460.77	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	685.13	J/molxK	775.25	Joback Method
cpg	699.76	J/molxK	809.64	Joback Method
cpg	713.41	J/molxK	844.03	Joback Method
cpg	726.08	J/molxK	878.43	Joback Method
cpg	737.79	J/molxK	912.82	Joback Method
cpg	748.56	J/molxK	947.21	Joback Method
cpg	758.39	J/molxK	981.60	Joback Method
dvisc	0.0006928	Paxs	460.77	Joback Method
dvisc	0.0003877	Paxs	513.18	Joback Method

dvisc	0.0002416	Paxs	565.60	Joback Method
dvisc	0.0001632	Paxs	618.01	Joback Method
dvisc	0.0001172	Paxs	670.42	Joback Method
dvisc	0.0000883	Paxs	722.84	Joback Method
dvisc	0.0000691	Paxs	775.25	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=C3035674&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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