Acetic acid, (2,4-dichlorophenoxy)-,2-octyl ester

Other names: 2,4-Dichlorophenoxyacetic acid, (1-methylheptyl) ester
Inchi: InChI=1S/C16H22Cl2O3/c1-3-4-5-6-7-12(2)21-16(19)11-20-15-9-8-13(17)10-14(15)18/h8
InchiKey: GJNVTNDAZUATRV-UHFFFAOYSA-N
Formula: C16H22Cl2O3
SMILES: CCCCCCC(C)OC(=O)COc1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 333.25
CAS: 1917-97-1

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	-5.70		Crippen Method
logp	5.274		Crippen Method
mcvol	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/mol×K	775.25	Joback Method
cpg	699.76	J/mol×K	809.64	Joback Method
cpg	713.41	J/mol×K	844.03	Joback Method
cpg	726.08	J/mol×K	878.43	Joback Method
cpg	737.79	J/mol×K	912.82	Joback Method
cpg	748.56	J/mol×K	947.21	Joback Method
cpg	758.39	J/mol×K	981.60	Joback Method
dvisc	0.0006928	Pa×s	460.77	Joback Method

dvisc	0.0003877	Pa×s	513.18	Joback Method
dvisc	0.0002416	Pa×s	565.60	Joback Method
dvisc	0.0001632	Pa×s	618.01	Joback Method
dvisc	0.0001172	Pa×s	670.42	Joback Method
dvisc	0.0000883	Pa×s	722.84	Joback Method
dvisc	0.0000691	Pa×s	775.25	Joback Method
hvapt	83.00	kJ/mol	517.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1917971&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
hvapt: Enthalpy of vaporization at a given temperature
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