Octyl (2,4-dichlorophenoxy)acetate

Other names: 2,4-Dichlorophenoxyacetic acid, octyl ester
Inchi: InChI=1S/C16H22Cl2O3/c1-2-3-4-5-6-7-10-20-16(19)12-21-15-9-8-13(17)11-14(15)18/h8
InchiKey: JWEDKKSQRXHXJD-UHFFFAOYSA-N
Formula: C16H22Cl2O3
SMILES: CCCCCCCCOC(=O)COc1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 333.25
CAS: 1928-44-5

Physical Properties

Property code	Value	Unit	Source
gf	-185.79	kJ/mol	Joback Method
hf	-568.48	kJ/mol	Joback Method
hfus	42.83	kJ/mol	Joback Method
hvap	75.15	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	5.276		Crippen Method
mcvol	250.330	ml/mol	McGowan Method
pc	1602.56	kPa	Joback Method
tb	775.69	K	Joback Method
tc	979.25	K	Joback Method
tf	475.77	K	Joback Method
vc	0.964	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.57	J/mol×K	775.69	Joback Method
cpg	699.00	J/mol×K	809.62	Joback Method
cpg	712.48	J/mol×K	843.54	Joback Method
cpg	725.03	J/mol×K	877.47	Joback Method
cpg	736.65	J/mol×K	911.40	Joback Method
cpg	747.36	J/mol×K	945.32	Joback Method
cpg	757.17	J/mol×K	979.25	Joback Method
dvisc	0.0006116	Pa×s	475.77	Joback Method

dvisc	0.0003652	Pa×s	525.76	Joback Method
dvisc	0.0002385	Pa×s	575.74	Joback Method
dvisc	0.0001667	Pa×s	625.73	Joback Method
dvisc	0.0001228	Pa×s	675.72	Joback Method
dvisc	0.0000944	Pa×s	725.70	Joback Method
dvisc	0.0000751	Pa×s	775.69	Joback Method
hvapt	87.90	kJ/mol	516.50	NIST Webbook

Sources

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=C1928445&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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