6-Methylheptyl (2,4,5-trichlorophenoxy)acetate

Inchi: InChI=1S/C16H21Cl3O3/c1-11(2)6-4-3-5-7-21-16(20)10-22-15-9-13(18)12(17)8-14(15)19
InchiKey: LRDPQMJVRJVAOH-UHFFFAOYSA-N
Formula: C16H21Cl3O3
SMILES: CC(C)CCCCCOC(=O)COc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]: 367.69
CAS: 116436-47-6

Physical Properties

Property code	Value	Unit	Source
gf	-209.79	kJ/mol	Joback Method
hf	-600.97	kJ/mol	Joback Method
hfus	43.11	kJ/mol	Joback Method
hvap	79.80	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	5.785		Crippen Method
mcvol	262.570	ml/mol	McGowan Method
pc	1547.57	kPa	Joback Method
tb	817.66	K	Joback Method
tc	1028.55	K	Joback Method
tf	503.21	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.62	J/mol×K	817.66	Joback Method
cpg	766.83	J/mol×K	993.40	Joback Method
cpg	757.34	J/mol×K	958.26	Joback Method
cpg	746.89	J/mol×K	923.11	Joback Method
cpg	735.46	J/mol×K	887.96	Joback Method
cpg	723.04	J/mol×K	852.81	Joback Method
cpg	775.36	J/mol×K	1028.55	Joback Method
dvisc	0.0000607	Pa×s	817.66	Joback Method
dvisc	0.0000763	Pa×s	765.25	Joback Method

dvisc	0.0000993	Pa×s	712.84	Joback Method
dvisc	0.0001347	Pa×s	660.43	Joback Method
dvisc	0.0001925	Pa×s	608.03	Joback Method
dvisc	0.0002944	Pa×s	555.62	Joback Method
dvisc	0.0004920	Pa×s	503.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116436476&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

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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