2,4-Dichlorophenoxyacetic acid, 3-(2-butoxyethoxy) propyl ester

Inchi: InChI=1S/C17H24Cl2O5/c1-2-3-7-21-10-11-22-8-4-9-23-17(20)13-24-16-6-5-14(18)12-15
InchiKey: RJKOZHSBYKYUJB-UHFFFAOYSA-N
Formula: C17H24Cl2O5
SMILES: CCCCOCCOCCCOC(=O)COc1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 379.27
CAS: 1928-57-0

Physical Properties

Property code	Value	Unit	Source
gf	-387.37	kJ/mol	Joback Method
hf	-853.56	kJ/mol	Joback Method
hfus	47.79	kJ/mol	Joback Method
hvap	82.19	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	4.139		Crippen Method
mcvol	276.160	ml/mol	McGowan Method
pc	1447.94	kPa	Joback Method
tb	843.41	K	Joback Method
tc	1046.59	K	Joback Method
tf	531.50	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.65	J/mol×K	843.41	Joback Method
cpg	810.53	J/mol×K	877.27	Joback Method
cpg	823.28	J/mol×K	911.14	Joback Method
cpg	834.90	J/mol×K	945.00	Joback Method
cpg	845.38	J/mol×K	978.86	Joback Method
cpg	854.70	J/mol×K	1012.73	Joback Method
cpg	862.85	J/mol×K	1046.59	Joback Method
dvisc	0.0002821	Pa×s	531.50	Joback Method
dvisc	0.0001729	Pa×s	583.49	Joback Method

dvisc	0.0001149	Pa×s	635.47	Joback Method
dvisc	0.0000811	Pa×s	687.45	Joback Method
dvisc	0.0000602	Pa×s	739.44	Joback Method
dvisc	0.0000465	Pa×s	791.42	Joback Method
dvisc	0.0000370	Pa×s	843.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1928570&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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