

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:	RJKOZHSHBYKYUJB-UHFFFAOYSA-N
Formula:	C17H24Cl2O5
SMILES:	CCCCOCCOCCOC(=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/molxK	843.41	Joback Method
cpg	810.53	J/molxK	877.27	Joback Method
cpg	823.28	J/molxK	911.14	Joback Method
cpg	834.90	J/molxK	945.00	Joback Method
cpg	845.38	J/molxK	978.86	Joback Method
cpg	854.70	J/molxK	1012.73	Joback Method
cpg	862.85	J/molxK	1046.59	Joback Method
dvisc	0.0002821	Paxs	531.50	Joback Method
dvisc	0.0001729	Paxs	583.49	Joback Method

dvisc	0.0001149	Paxs	635.47	Joback Method
dvisc	0.0000811	Paxs	687.45	Joback Method
dvisc	0.0000602	Paxs	739.44	Joback Method
dvisc	0.0000465	Paxs	791.42	Joback Method
dvisc	0.0000370	Paxs	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
mccvol:	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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