

Diglycolic acid, 2,6-dichlorophenyl hexyl ester

Inchi:	InChI=1S/C16H20Cl2O5/c1-2-3-4-5-9-22-14(19)10-21-11-15(20)23-16-12(17)7-6-8-13(16)
InchiKey:	VTSUYHZBSBBPGK-UHFFFAOYSA-N
Formula:	C16H20Cl2O5
SMILES:	CCCCCOC(=O)COCC(=O)Oc1c(Cl)cccc1Cl
Mol. weight [g/mol]:	363.23

Physical Properties

Property code	Value	Unit	Source
gf	-419.71	kJ/mol	Joback Method
hf	-813.28	kJ/mol	Joback Method
hfus	45.61	kJ/mol	Joback Method
hvap	84.30	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	4.039		Crippen Method
mvol	257.770	ml/mol	McGowan Method
pc	1663.26	kPa	Joback Method
rinpol	2993.00		NIST Webbook
rinpol	2993.00		NIST Webbook
tb	851.98	K	Joback Method
tc	1062.16	K	Joback Method
tf	547.93	K	Joback Method
vc	0.988	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	725.51	J/molxK	851.98	Joback Method
cpg	776.36	J/molxK	1027.13	Joback Method
cpg	768.36	J/molxK	992.10	Joback Method
cpg	759.27	J/molxK	957.07	Joback Method
cpg	749.10	J/molxK	922.04	Joback Method
cpg	737.85	J/molxK	887.01	Joback Method
cpg	783.27	J/molxK	1062.16	Joback Method
dvisc	0.0000547	Paxs	851.98	Joback Method

dvisc	0.0000681	Paxs	801.31	Joback Method
dvisc	0.0000873	Paxs	750.63	Joback Method
dvisc	0.0001160	Paxs	699.96	Joback Method
dvisc	0.0001612	Paxs	649.28	Joback Method
dvisc	0.0002368	Paxs	598.61	Joback Method
dvisc	0.0003735	Paxs	547.93	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382301&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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