

Diglycolic acid, butyl 2-chlorophenyl ester

Inchi:	InChI=1S/C14H17ClO5/c1-2-3-8-19-13(16)9-18-10-14(17)20-12-7-5-4-6-11(12)15/h4-7H
InchiKey:	DLYBAUBUTXXIFN-UHFFFAOYSA-N
Formula:	C14H17ClO5
SMILES:	CCCCOC(=O)COCC(=O)Oc1ccccc1Cl
Mol. weight [g/mol]:	300.74

Physical Properties

Property code	Value	Unit	Source
gf	-414.99	kJ/mol	Joback Method
hf	-744.79	kJ/mol	Joback Method
hfus	36.63	kJ/mol	Joback Method
hvap	74.80	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.605		Crippen Method
mvol	217.350	ml/mol	McGowan Method
pc	2051.17	kPa	Joback Method
rinpol	2582.00		NIST Webbook
rinpol	2582.00		NIST Webbook
tb	763.81	K	Joback Method
tc	971.80	K	Joback Method
tf	482.95	K	Joback Method
vc	0.827	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.22	J/molxK	763.81	Joback Method
cpg	647.66	J/molxK	937.14	Joback Method
cpg	638.48	J/molxK	902.47	Joback Method
cpg	628.35	J/molxK	867.81	Joback Method
cpg	617.25	J/molxK	833.14	Joback Method
cpg	605.21	J/molxK	798.48	Joback Method
cpg	655.88	J/molxK	971.80	Joback Method
dvisc	0.0000820	Paxs	763.81	Joback Method

dvisc	0.0001028	Paxs	717.00	Joback Method
dvisc	0.0001330	Paxs	670.19	Joback Method
dvisc	0.0001788	Paxs	623.38	Joback Method
dvisc	0.0002521	Paxs	576.57	Joback Method
dvisc	0.0003779	Paxs	529.76	Joback Method
dvisc	0.0006127	Paxs	482.95	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=U381971&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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