

Diglycolic acid, butyl 2,4-dichlorophenyl ester

Inchi:	InChI=1S/C14H16Cl2O5/c1-2-3-6-20-13(17)8-19-9-14(18)21-12-5-4-10(15)7-11(12)16/h
InchiKey:	SBZBCYJTJOIIEC-UHFFFAOYSA-N
Formula:	C14H16Cl2O5
SMILES:	CCCCOC(=O)COCC(=O)Oc1ccc(Cl)cc1Cl
Mol. weight [g/mol]:	335.18

Physical Properties

Property code	Value	Unit	Source
gf	-436.55	kJ/mol	Joback Method
hf	-772.00	kJ/mol	Joback Method
hfus	40.43	kJ/mol	Joback Method
hvap	79.85	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.259		Crippen Method
mvol	229.590	ml/mol	McGowan Method
pc	1957.87	kPa	Joback Method
rinpol	2957.00		NIST Webbook
rinpol	2957.00		NIST Webbook
tb	806.22	K	Joback Method
tc	1018.57	K	Joback Method
tf	525.39	K	Joback Method
vc	0.875	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.67	J/molxK	806.22	Joback Method
cpg	626.44	J/molxK	841.61	Joback Method
cpg	637.25	J/molxK	877.00	Joback Method
cpg	647.07	J/molxK	912.39	Joback Method
cpg	655.89	J/molxK	947.78	Joback Method
cpg	663.71	J/molxK	983.17	Joback Method
cpg	670.52	J/molxK	1018.57	Joback Method
dvisc	0.0004517	Paxs	525.39	Joback Method

dvisc	0.0002939	Paxs	572.19	Joback Method
dvisc	0.0002041	Paxs	619.00	Joback Method
dvisc	0.0001491	Paxs	665.81	Joback Method
dvisc	0.0001136	Paxs	712.61	Joback Method
dvisc	0.0000895	Paxs	759.41	Joback Method
dvisc	0.0000724	Paxs	806.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381987&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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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