

Diglycolic acid, 2,3-dichlorophenyl isobutyl ester

Inchi:	InChI=1S/C14H16Cl2O5/c1-9(2)6-20-12(17)7-19-8-13(18)21-11-5-3-4-10(15)14(11)16/h3
InchiKey:	CPVONGRCRPNNBT-UHFFFAOYSA-N
Formula:	C14H16Cl2O5
SMILES:	CC(C)COC(=O)COCC(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	335.18

Physical Properties

Property code	Value	Unit	Source
gf	-438.99	kJ/mol	Joback Method
hf	-777.28	kJ/mol	Joback Method
hfus	36.91	kJ/mol	Joback Method
hvap	79.46	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	3.115		Crippen Method
mcvol	229.590	ml/mol	McGowan Method
pc	1971.80	kPa	Joback Method
rinpola	2746.00		NIST Webbook
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tb	805.78	K	Joback Method
tc	1021.07	K	Joback Method
tf	510.39	K	Joback Method
vc	0.870	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	615.26	J/molxK	805.78	Joback Method
cpg	627.20	J/molxK	841.66	Joback Method
cpg	638.12	J/molxK	877.54	Joback Method
cpg	648.01	J/molxK	913.43	Joback Method
cpg	656.87	J/molxK	949.31	Joback Method
cpg	664.69	J/molxK	985.19	Joback Method
cpg	671.46	J/molxK	1021.07	Joback Method
dvisc	0.0004965	Paxs	510.39	Joback Method

dvisc	0.0003065	Paxs	559.62	Joback Method
dvisc	0.0002046	Paxs	608.85	Joback Method
dvisc	0.0001450	Paxs	658.09	Joback Method
dvisc	0.0001079	Paxs	707.32	Joback Method
dvisc	0.0000834	Paxs	756.55	Joback Method
dvisc	0.0000665	Paxs	805.78	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=U382089&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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