

Diglycolic acid, 2,3-dichlorophenyl ethyl ester

Inchi:	InChI=1S/C12H12Cl2O5/c1-2-18-10(15)6-17-7-11(16)19-9-5-3-4-8(13)12(9)14/h3-5H,2,6
InchiKey:	AOQJXIWCPYFGGN-UHFFFAOYSA-N
Formula:	C12H12Cl2O5
SMILES:	CCOC(=O)COCC(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	307.13

Physical Properties

Property code	Value	Unit	Source
gf	-453.39	kJ/mol	Joback Method
hf	-730.72	kJ/mol	Joback Method
hfus	35.25	kJ/mol	Joback Method
hvap	75.40	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.478		Crippen Method
mvol	201.410	ml/mol	McGowan Method
pc	2338.29	kPa	Joback Method
rinpol	2558.00		NIST Webbook
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tb	760.46	K	Joback Method
tc	977.36	K	Joback Method
tf	502.85	K	Joback Method
vc	0.763	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.79	J/molxK	760.46	Joback Method
cpg	553.85	J/molxK	941.21	Joback Method
cpg	546.45	J/molxK	905.06	Joback Method
cpg	538.12	J/molxK	868.91	Joback Method
cpg	528.89	J/molxK	832.76	Joback Method
cpg	518.77	J/molxK	796.61	Joback Method
cpg	560.32	J/molxK	977.36	Joback Method
dvisc	0.0000948	Paxs	760.46	Joback Method

dvisc	0.0001161	Paxs	717.53	Joback Method
dvisc	0.0001458	Paxs	674.59	Joback Method
dvisc	0.0001890	Paxs	631.65	Joback Method
dvisc	0.0002543	Paxs	588.72	Joback Method
dvisc	0.0003586	Paxs	545.79	Joback Method
dvisc	0.0005363	Paxs	502.85	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U382087&Units=SI

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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