

Diglycolic acid, 3-chlorophenyl propyl ester

Inchi:	InChI=1S/C13H15ClO5/c1-2-6-18-12(15)8-17-9-13(16)19-11-5-3-4-10(14)7-11/h3-5,7H,2
InchiKey:	RXSYAOKEBWMLIF-UHFFFAOYSA-N
Formula:	C13H15ClO5
SMILES:	CCCOC(=O)COCC(=O)Oc1cccc(Cl)c1
Mol. weight [g/mol]:	286.71

Physical Properties

Property code	Value	Unit	Source
gf	-423.41	kJ/mol	Joback Method
hf	-724.15	kJ/mol	Joback Method
hfus	34.04	kJ/mol	Joback Method
hvap	72.58	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.215		Crippen Method
mcvol	203.260	ml/mol	McGowan Method
pc	2241.88	kPa	Joback Method
rinpol	2475.00		NIST Webbook
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tb	740.93	K	Joback Method
tc	951.16	K	Joback Method
tf	471.68	K	Joback Method
vc	0.770	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.67	J/molxK	740.93	Joback Method
cpg	551.27	J/molxK	775.97	Joback Method
cpg	562.97	J/molxK	811.01	Joback Method
cpg	573.76	J/molxK	846.04	Joback Method
cpg	583.64	J/molxK	881.08	Joback Method
cpg	592.60	J/molxK	916.12	Joback Method
cpg	600.63	J/molxK	951.16	Joback Method
dvisc	0.0006652	Paxs	471.68	Joback Method

dvisc	0.0004162	Paxs	516.56	Joback Method
dvisc	0.0002806	Paxs	561.43	Joback Method
dvisc	0.0002006	Paxs	606.31	Joback Method
dvisc	0.0001502	Paxs	651.18	Joback Method
dvisc	0.0001167	Paxs	696.06	Joback Method
dvisc	0.0000935	Paxs	740.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381766&Units=SI
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

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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