

Diglycolic acid, 4-chlorophenyl ethyl ester

Inchi:	InChI=1S/C12H13ClO5/c1-2-17-11(14)7-16-8-12(15)18-10-5-3-9(13)4-6-10/h3-6H,2,7-8H
InchiKey:	IMGQYRVGMOBLRW-UHFFFAOYSA-N
Formula:	C12H13ClO5
SMILES:	CCOC(=O)COCC(=O)Oc1ccc(Cl)cc1
Mol. weight [g/mol]:	272.68

Physical Properties

Property code	Value	Unit	Source
gf	-431.83	kJ/mol	Joback Method
hf	-703.51	kJ/mol	Joback Method
hfus	31.45	kJ/mol	Joback Method
hvap	70.35	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	1.825		Crippen Method
mvol	189.170	ml/mol	McGowan Method
pc	2460.47	kPa	Joback Method
rinpol	2376.00		NIST Webbook
rinpol	2376.00		NIST Webbook
tb	718.05	K	Joback Method
tc	931.00	K	Joback Method
tf	460.41	K	Joback Method
vc	0.715	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.30	J/molxK	718.05	Joback Method
cpg	498.43	J/molxK	753.54	Joback Method
cpg	509.71	J/molxK	789.03	Joback Method
cpg	520.13	J/molxK	824.53	Joback Method
cpg	529.68	J/molxK	860.02	Joback Method
cpg	538.35	J/molxK	895.51	Joback Method
cpg	546.13	J/molxK	931.00	Joback Method
dvisc	0.0007181	Paxs	460.41	Joback Method

dvisc	0.0004558	Paxs	503.35	Joback Method
dvisc	0.0003108	Paxs	546.29	Joback Method
dvisc	0.0002241	Paxs	589.23	Joback Method
dvisc	0.0001689	Paxs	632.17	Joback Method
dvisc	0.0001320	Paxs	675.11	Joback Method
dvisc	0.0001062	Paxs	718.05	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=U381775&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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