Diglycolic acid, 4-chloro-2-acetylphenyl ethyl ester

Inchi: InChI=1S/C14H15ClO6/c1-3-20-13(17)7-19-8-14(18)21-12-5-4-10(15)6-11(12)9(2)16/h4-

InchiKey: NKDMVZZPZMZBKP-UHFFFAOYSA-N

Formula: C14H15ClO6

SMILES: CCOC(=O)COCC(=O)Oc1ccc(Cl)cc1C(C)=O

Mol. weight [g/mol]: 314.72

Physical Properties

Property code	Value	Unit	Source
gf	-553.54	kJ/mol	Joback Method
hf	-868.84	kJ/mol	Joback Method
hfus	37.84	kJ/mol	Joback Method
hvap	82.21	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.028		Crippen Method
mcvol	218.920	ml/mol	McGowan Method
pc	2143.35	kPa	Joback Method
rinpol	2644.00		NIST Webbook
rinpol	2644.00		NIST Webbook
tb	822.66	K	Joback Method
tc	1037.77	K	Joback Method
tf	545.40	K	Joback Method
vc	0.833	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.53	J/mol×K	822.66	Joback Method
cpg	613.74	J/mol×K	858.51	Joback Method
cpg	623.92	J/mol×K	894.36	Joback Method
cpg	633.06	J/mol×K	930.21	Joback Method
cpg	641.15	J/mol×K	966.07	Joback Method
cpg	648.17	J/mol×K	1001.92	Joback Method
cpg	654.11	J/mol×K	1037.77	Joback Method
dvisc	0.0004629	Pa×s	545.40	Joback Method

dvisc	0.0003084	Pa×s	591.61	Joback Method
dvisc	0.0002179	Pa×s	637.82	Joback Method
dvisc	0.0001614	Pa×s	684.03	Joback Method
dvisc	0.0001242	Pa×s	730.24	Joback Method
dvisc	0.0000985	Pa×s	776.45	Joback Method
dvisc	0.0000803	Pa×s	822.66	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=U382702&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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