Diglycolic acid, 4-acetylphenyl ethyl ester

Inchi: InChI=1S/C14H16O6/c1-3-19-13(16)8-18-9-14(17)20-12-6-4-11(5-7-12)10(2)15/h4-7H,3,
InchiKey: HIBQMBSYECRFTP-UHFFFAOYSA-N
Formula: C14H16O6
SMILES: CCOC(=O)COCC(=O)Oc1ccc(C(C)=O)cc1
Mol. weight [g/mol]: 280.27

Physical Properties

Property code	Value	Unit	Source
gf	-531.98	kJ/mol	Joback Method
hf	-841.63	kJ/mol	Joback Method
hfus	34.03	kJ/mol	Joback Method
hvap	77.16	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	1.374		Crippen Method
mcvol	206.680	ml/mol	McGowan Method
pc	2250.40	kPa	Joback Method
rinpol	2673.00		NIST Webbook
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tb	780.25	K	Joback Method
tc	991.06	K	Joback Method
tf	502.96	K	Joback Method
vc	0.783	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.06	J/mol×K	780.25	Joback Method
cpg	633.43	J/mol×K	955.92	Joback Method
cpg	624.96	J/mol×K	920.79	Joback Method
cpg	615.49	J/mol×K	885.65	Joback Method
cpg	605.00	J/mol×K	850.52	Joback Method
cpg	593.53	J/mol×K	815.38	Joback Method
cpg	640.86	J/mol×K	991.06	Joback Method
dvisc	0.0000903	Pa×s	780.25	Joback Method

dvisc	0.0001124	Pa×s	734.04	Joback Method
dvisc	0.0001441	Pa×s	687.82	Joback Method
dvisc	0.0001915	Pa×s	641.61	Joback Method
dvisc	0.0002660	Pa×s	595.39	Joback Method
dvisc	0.0003905	Pa×s	549.18	Joback Method
dvisc	0.0006150	Pa×s	502.96	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=U382698&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