Diglycolic acid, 2-acetylphenyl propyl ester

Inchi: InChI=1S/C15H18O6/c1-3-8-20-14(17)9-19-10-15(18)21-13-7-5-4-6-12(13)11(2)16/h4-7H
InchiKey: ATXHVBGZXIEPKC-UHFFFAOYSA-N
Formula: C15H18O6
SMILES: CCCOC(=O)COCC(=O)Oc1ccccc1C(C)=O
Mol. weight [g/mol]: 294.30

Physical Properties

Property code	Value	Unit	Source
gf	-523.56	kJ/mol	Joback Method
hf	-862.27	kJ/mol	Joback Method
hfus	36.62	kJ/mol	Joback Method
hvap	79.39	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	1.764		Crippen Method
mcvol	220.770	ml/mol	McGowan Method
pc	2058.62	kPa	Joback Method
rinpol	2475.00		NIST Webbook
tb	803.13	K	Joback Method
tc	1012.23	K	Joback Method
tf	514.23	K	Joback Method
vc	0.840	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	635.75	J/mol×K	803.13	Joback Method
cpg	689.18	J/mol×K	977.38	Joback Method
cpg	680.59	J/mol×K	942.53	Joback Method
cpg	670.95	J/mol×K	907.68	Joback Method
cpg	660.26	J/mol×K	872.83	Joback Method
cpg	648.52	J/mol×K	837.98	Joback Method
cpg	696.70	J/mol×K	1012.23	Joback Method
dvisc	0.0000791	Pa×s	803.13	Joback Method
dvisc	0.0000989	Pa×s	754.98	Joback Method

dvisc	0.0001274	Pa×s	706.83	Joback Method
dvisc	0.0001704	Pa×s	658.68	Joback Method
dvisc	0.0002385	Pa×s	610.53	Joback Method
dvisc	0.0003537	Pa×s	562.38	Joback Method
dvisc	0.0005647	Pa×s	514.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382717&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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