Diglycolic acid, 2-acetylphenyl butyl ester

Inchi: InChI=1S/C16H20O6/c1-3-4-9-21-15(18)10-20-11-16(19)22-14-8-6-5-7-13(14)12(2)17/h5
InchiKey: CTNVLYZEVOPPNW-UHFFFAOYSA-N
Formula: C16H20O6
SMILES: CCCCOC(=O)COCC(=O)Oc1ccccc1C(C)=O
Mol. weight [g/mol]: 308.33

Physical Properties

Property code	Value	Unit	Source
gf	-515.14	kJ/mol	Joback Method
hf	-882.91	kJ/mol	Joback Method
hfus	39.21	kJ/mol	Joback Method
hvap	81.62	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.154		Crippen Method
mcvol	234.860	ml/mol	McGowan Method
pc	1890.36	kPa	Joback Method
rinpol	2719.00		NIST Webbook
rinpol	2719.00		NIST Webbook
tb	826.01	K	Joback Method
tc	1034.00	K	Joback Method
tf	525.50	K	Joback Method
vc	0.895	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	691.41	J/mol×K	826.01	Joback Method
cpg	704.43	J/mol×K	860.67	Joback Method
cpg	716.36	J/mol×K	895.34	Joback Method
cpg	727.21	J/mol×K	930.00	Joback Method
cpg	736.96	J/mol×K	964.67	Joback Method
cpg	745.62	J/mol×K	999.33	Joback Method
cpg	753.18	J/mol×K	1034.00	Joback Method
dvisc	0.0005159	Pa×s	525.50	Joback Method

dvisc	0.0003189	Pa×s	575.59	Joback Method
dvisc	0.0002130	Pa×s	625.67	Joback Method
dvisc	0.0001510	Pa×s	675.75	Joback Method
dvisc	0.0001122	Pa×s	725.84	Joback Method
dvisc	0.0000867	Pa×s	775.92	Joback Method
dvisc	0.0000691	Pa×s	826.01	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382719&Units=SI

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