Diglycolic acid, 4-acetylphenyl hexyl ester

Inchi: InChI=1S/C18H24O6/c1-3-4-5-6-11-23-17(20)12-22-13-18(21)24-16-9-7-15(8-10-16)14(2
InchiKey: QCJQTTMIKHEZMC-UHFFFAOYSA-N
Formula: C18H24O6
SMILES: CCCCCCOC(=O)COCC(=O)Oc1ccc(C(C)=O)cc1
Mol. weight [g/mol]: 336.38

Physical Properties

Property code	Value	Unit	Source
gf	-498.30	kJ/mol	Joback Method
hf	-924.19	kJ/mol	Joback Method
hfus	44.39	kJ/mol	Joback Method
hvap	86.07	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	2.935		Crippen Method
mcvol	263.040	ml/mol	McGowan Method
pc	1610.29	kPa	Joback Method
rinpol	3171.00		NIST Webbook
rinpol	3171.00		NIST Webbook
tb	871.77	K	Joback Method
tc	1079.52	K	Joback Method
tf	548.04	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	805.26	J/mol×K	871.77	Joback Method
cpg	860.41	J/mol×K	1044.90	Joback Method
cpg	851.75	J/mol×K	1010.27	Joback Method
cpg	841.91	J/mol×K	975.65	Joback Method
cpg	830.89	J/mol×K	941.02	Joback Method
cpg	818.67	J/mol×K	906.40	Joback Method
cpg	867.88	J/mol×K	1079.52	Joback Method
dvisc	0.0000522	Pa×s	871.77	Joback Method

dvisc	0.0000660	Pa×s	817.82	Joback Method
dvisc	0.0000862	Pa×s	763.86	Joback Method
dvisc	0.0001173	Pa×s	709.90	Joback Method
dvisc	0.0001678	Pa×s	655.95	Joback Method
dvisc	0.0002561	Pa×s	602.00	Joback Method
dvisc	0.0004247	Pa×s	548.04	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=U382701&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