Diglycolic acid, 4-acetylphenyl pentyl ester

Inchi: InChI=1S/C17H22O6/c1-3-4-5-10-22-16(19)11-21-12-17(20)23-15-8-6-14(7-9-15)13(2)18

InchiKey: IFUMQIBOZFURLN-UHFFFAOYSA-N

Formula: C17H22O6

SMILES: CCCCCOC(=O)COCC(=O)Oc1ccc(C(C)=O)cc1

Mol. weight [g/mol]: 322.35

Physical Properties

Property code	Value	Unit	Source
gf	-506.72	kJ/mol	Joback Method
hf	-903.55	kJ/mol	Joback Method
hfus	41.80	kJ/mol	Joback Method
hvap	83.84	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	2.545		Crippen Method
mcvol	248.950	ml/mol	McGowan Method
pc	1741.91	kPa	Joback Method
rinpol	3048.00		NIST Webbook
rinpol	3048.00		NIST Webbook
tb	848.89	K	Joback Method
tc	1056.41	K	Joback Method
tf	536.77	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	747.93	J/mol×K	848.89	Joback Method
cpg	761.17	J/mol×K	883.48	Joback Method
cpg	773.26	J/mol×K	918.06	Joback Method
cpg	784.21	J/mol×K	952.65	Joback Method
cpg	794.03	J/mol×K	987.24	Joback Method
cpg	802.71	J/mol×K	1021.83	Joback Method
cpg	810.25	J/mol×K	1056.41	Joback Method
dvisc	0.0004691	Pa×s	536.77	Joback Method

dvisc	0.0002864	Pa×s	588.79	Joback Method
dvisc	0.0001894	Pa×s	640.81	Joback Method
dvisc	0.0001333	Pa×s	692.83	Joback Method
dvisc	0.0000985	Pa×s	744.85	Joback Method
dvisc	0.0000758	Pa×s	796.87	Joback Method
dvisc	0.0000602	Pa×s	848.89	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=U382700&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