Diglycolic acid, 2-acetylphenyl heptyl ester

Inchi: InChI=1S/C19H26O6/c1-3-4-5-6-9-12-24-18(21)13-23-14-19(22)25-17-11-8-7-10-16(17)1
InchiKey: GTFYSMDDWGPWNS-UHFFFAOYSA-N
Formula: C19H26O6
SMILES: CCCCCCCOC(=O)COCC(=O)Oc1ccccc1C(C)=O
Mol. weight [g/mol]: 350.41

Physical Properties

Property code	Value	Unit	Source
gf	-489.88	kJ/mol	Joback Method
hf	-944.83	kJ/mol	Joback Method
hfus	46.98	kJ/mol	Joback Method
hvap	88.29	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.325		Crippen Method
mcvol	277.130	ml/mol	McGowan Method
pc	1493.04	kPa	Joback Method
rinpol	3100.00		NIST Webbook
tb	894.65	K	Joback Method
tc	1103.37	K	Joback Method
tf	559.31	K	Joback Method
vc	1.063	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	863.32	J/mol×K	894.65	Joback Method
cpg	876.88	J/mol×K	929.44	Joback Method
cpg	889.19	J/mol×K	964.22	Joback Method
cpg	900.25	J/mol×K	999.01	Joback Method
cpg	910.07	J/mol×K	1033.80	Joback Method
cpg	918.65	J/mol×K	1068.59	Joback Method
cpg	926.01	J/mol×K	1103.37	Joback Method
dvisc	0.0003829	Pa×s	559.31	Joback Method
dvisc	0.0002282	Pa×s	615.20	Joback Method

dvisc	0.0001482	Pa×s	671.09	Joback Method
dvisc	0.0001029	Pa×s	726.98	Joback Method
dvisc	0.0000753	Pa×s	782.87	Joback Method
dvisc	0.0000574	Pa×s	838.76	Joback Method
dvisc	0.0000453	Pa×s	894.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382723&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