Diglycolic acid, 2-acetylphenyl octyl ester

Inchi: InChI=1S/C20H28O6/c1-3-4-5-6-7-10-13-25-19(22)14-24-15-20(23)26-18-12-9-8-11-17(1
InchiKey: KNUYXZORSDYQKX-UHFFFAOYSA-N
Formula: C20H28O6
SMILES: CCCCCCCCOC(=O)COCC(=O)Oc1ccccc1C(C)=O
Mol. weight [g/mol]: 364.43

Physical Properties

Property code	Value	Unit	Source
gf	-481.46	kJ/mol	Joback Method
hf	-965.47	kJ/mol	Joback Method
hfus	49.57	kJ/mol	Joback Method
hvap	90.52	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	3.715		Crippen Method
mcvol	291.220	ml/mol	McGowan Method
pc	1388.15	kPa	Joback Method
rinpol	3222.00		NIST Webbook
rinpol	3222.00		NIST Webbook
tb	917.53	K	Joback Method
tc	1128.02	K	Joback Method
tf	570.58	K	Joback Method
vc	1.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	922.03	J/mol×K	917.53	Joback Method
cpg	977.41	J/mol×K	1092.94	Joback Method
cpg	968.94	J/mol×K	1057.86	Joback Method
cpg	959.17	J/mol×K	1022.78	Joback Method
cpg	948.11	J/mol×K	987.69	Joback Method
cpg	935.73	J/mol×K	952.61	Joback Method
cpg	984.59	J/mol×K	1128.02	Joback Method
dvisc	0.0000391	Pa×s	917.53	Joback Method

dvisc	0.0000497	Pa×s	859.70	Joback Method
dvisc	0.0000655	Pa×s	801.88	Joback Method
dvisc	0.0000900	Pa×s	744.05	Joback Method
dvisc	0.0001305	Pa×s	686.23	Joback Method
dvisc	0.0002026	Pa×s	628.40	Joback Method
dvisc	0.0003440	Pa×s	570.58	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=U382724&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