Diglycolic acid, 2-acetylphenyl decyl ester

Inchi: InChI=1S/C22H32O6/c1-3-4-5-6-7-8-9-12-15-27-21(24)16-26-17-22(25)28-20-14-11-10-1
InchiKey: UNUDXDLNBUVECV-UHFFFAOYSA-N
Formula: C22H32O6
SMILES: CCCCCCCCCCOC(=O)COCC(=O)Oc1ccccc1C(C)=O
Mol. weight [g/mol]: 392.49

Physical Properties

Property code	Value	Unit	Source
gf	-464.62	kJ/mol	Joback Method
hf	-1006.75	kJ/mol	Joback Method
hfus	54.75	kJ/mol	Joback Method
hvap	94.97	kJ/mol	Joback Method
log10ws	-5.42		Crippen Method
logp	4.495		Crippen Method
mcvol	319.400	ml/mol	McGowan Method
pc	1208.99	kPa	Joback Method
rinpol	3442.00		NIST Webbook
rinpol	3442.00		NIST Webbook
tb	963.29	K	Joback Method
tc	1179.95	K	Joback Method
tf	593.12	K	Joback Method
vc	1.232	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1041.16	J/mol×K	963.29	Joback Method
cpg	1055.10	J/mol×K	999.40	Joback Method
cpg	1067.56	J/mol×K	1035.51	Joback Method
cpg	1078.55	J/mol×K	1071.62	Joback Method
cpg	1088.09	J/mol×K	1107.73	Joback Method
cpg	1096.19	J/mol×K	1143.84	Joback Method
cpg	1102.88	J/mol×K	1179.95	Joback Method
dvisc	0.0002747	Pa×s	593.12	Joback Method

dvisc	0.0001583	Pa×s	654.82	Joback Method
dvisc	0.0001003	Pa×s	716.51	Joback Method
dvisc	0.0000684	Pa×s	778.20	Joback Method
dvisc	0.0000493	Pa×s	839.90	Joback Method
dvisc	0.0000371	Pa×s	901.59	Joback Method
dvisc	0.0000290	Pa×s	963.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382726&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