Diglycolic acid, 2-acetylphenyl undecyl ester

Inchi: InChI=1S/C23H34O6/c1-3-4-5-6-7-8-9-10-13-16-28-22(25)17-27-18-23(26)29-21-15-12-1

InchiKey: CUHFUZCEHQJNEU-UHFFFAOYSA-N

Formula: C23H34O6

SMILES: CCCCCCCCCCCOC(=O)COCC(=O)Oc1ccccc1C(C)=O

Mol. weight [g/mol]: 406.51

Physical Properties

Property code	Value	Unit	Source
gf	-456.20	kJ/mol	Joback Method
hf	-1027.39	kJ/mol	Joback Method
hfus	57.34	kJ/mol	Joback Method
hvap	97.20	kJ/mol	Joback Method
log10ws	-5.84		Crippen Method
logp	4.885		Crippen Method
mcvol	333.490	ml/mol	McGowan Method
pc	1132.15	kPa	Joback Method
rinpol	3560.00		NIST Webbook
rinpol	3560.00		NIST Webbook
tb	986.17	K	Joback Method
tc	1207.35	K	Joback Method
tf	604.39	K	Joback Method
vc	1.288	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1101.45	J/mol×K	986.17	Joback Method
cpg	1156.11	J/mol×K	1170.49	Joback Method
cpg	1148.26	J/mol×K	1133.63	Joback Method
cpg	1138.89	J/mol×K	1096.76	Joback Method
cpg	1127.98	J/mol×K	1059.90	Joback Method
cpg	1115.51	J/mol×K	1023.03	Joback Method
cpg	1162.46	J/mol×K	1207.35	Joback Method
dvisc	0.0000249	Pa×s	986.17	Joback Method

dvisc	0.0000320	Pa×s	922.54	Joback Method
dvisc	0.0000426	Pa×s	858.91	Joback Method
dvisc	0.0000594	Pa×s	795.28	Joback Method
dvisc	0.0000876	Pa×s	731.65	Joback Method
dvisc	0.0001394	Pa×s	668.02	Joback Method
dvisc	0.0002443	Pa×s	604.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382727&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