Diethylmalonic acid, 4-acetylphenyl octyl ester

Inchi: InChI=1S/C23H34O5/c1-5-8-9-10-11-12-17-27-21(25)23(6-2,7-3)22(26)28-20-15-13-19(1
InchiKey: MOTSDYSVCKWWHT-UHFFFAOYSA-N
Formula: C23H34O5
SMILES: CCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(C(C)=O)cc1
Mol. weight [g/mol]: 390.51

Physical Properties

Property code	Value	Unit	Source
gf	-348.36	kJ/mol	Joback Method
hf	-903.92	kJ/mol	Joback Method
hfus	48.74	kJ/mol	Joback Method
hvap	93.49	kJ/mol	Joback Method
log10ws	-6.51		Crippen Method
logp	5.505		Crippen Method
mcvol	327.620	ml/mol	McGowan Method
pc	1160.08	kPa	Joback Method
rinpol	2705.00		NIST Webbook
rinpol	2705.00		NIST Webbook
tb	960.52	K	Joback Method
tc	1178.29	K	Joback Method
tf	584.58	K	Joback Method
vc	1.258	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1073.70	J/mol×K	960.52	Joback Method
cpg	1088.63	J/mol×K	996.81	Joback Method
cpg	1102.27	J/mol×K	1033.11	Joback Method
cpg	1114.66	J/mol×K	1069.40	Joback Method
cpg	1125.88	J/mol×K	1105.70	Joback Method
cpg	1135.96	J/mol×K	1141.99	Joback Method
cpg	1144.98	J/mol×K	1178.29	Joback Method
dvisc	0.0003027	Pa×s	584.58	Joback Method

dvisc	0.0001645	Pa×s	647.24	Joback Method
dvisc	0.0000996	Pa×s	709.89	Joback Method
dvisc	0.0000654	Pa×s	772.55	Joback Method
dvisc	0.0000457	Pa×s	835.21	Joback Method
dvisc	0.0000336	Pa×s	897.86	Joback Method
dvisc	0.0000257	Pa×s	960.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370086&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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