Dimethylmalonic acid, 4-acetylphenyl tridecyl ester

Inchi: InChI=1S/C26H40O5/c1-5-6-7-8-9-10-11-12-13-14-15-20-30-24(28)26(3,4)25(29)31-23-1
InchiKey: NUQIMPDVRJHXBT-UHFFFAOYSA-N
Formula: C26H40O5
SMILES: CCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1ccc(C(C)=O)cc1
Mol. weight [g/mol]: 432.59

Physical Properties

Property code	Value	Unit	Source
gf	-323.10	kJ/mol	Joback Method
hf	-965.84	kJ/mol	Joback Method
hfus	56.51	kJ/mol	Joback Method
hvap	100.17	kJ/mol	Joback Method
log10ws	-7.76		Crippen Method
logp	6.675		Crippen Method
mcvol	369.890	ml/mol	McGowan Method
pc	962.08	kPa	Joback Method
rinpol	3007.00		NIST Webbook
tb	1029.16	K	Joback Method
tc	1260.40	K	Joback Method
tf	618.39	K	Joback Method
vc	1.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1257.49	J/mol×K	1029.16	Joback Method
cpg	1273.08	J/mol×K	1067.70	Joback Method
cpg	1287.20	J/mol×K	1106.24	Joback Method
cpg	1299.91	J/mol×K	1144.78	Joback Method
cpg	1311.30	J/mol×K	1183.32	Joback Method
cpg	1321.45	J/mol×K	1221.86	Joback Method
cpg	1330.44	J/mol×K	1260.40	Joback Method
dvisc	0.0002066	Pa×s	618.39	Joback Method
dvisc	0.0001090	Pa×s	686.85	Joback Method

dvisc	0.0000646	Pa×s	755.31	Joback Method
dvisc	0.0000418	Pa×s	823.77	Joback Method
dvisc	0.0000289	Pa×s	892.24	Joback Method
dvisc	0.0000210	Pa×s	960.70	Joback Method
dvisc	0.0000160	Pa×s	1029.16	Joback Method

Sources

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=U363706&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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