Dimethylmalonic acid, 4-acetylphenyl pentadecyl ester

Inchi: InChI=1S/C28H44O5/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-22-32-26(30)28(3,4)27(31)3

InchiKey: HDUNLWAMDYZZKU-UHFFFAOYSA-N

Formula: C28H44O5

SMILES: CCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1ccc(C(C)=O)cc1

Mol. weight [g/mol]: 460.65

Physical Properties

Property code	Value	Unit	Source
gf	-306.26	kJ/mol	Joback Method
hf	-1007.12	kJ/mol	Joback Method
hfus	61.69	kJ/mol	Joback Method
hvap	104.62	kJ/mol	Joback Method
log10ws	-8.60		Crippen Method
logp	7.455		Crippen Method
mcvol	398.070	ml/mol	McGowan Method
pc	856.97	kPa	Joback Method
rinpol	3223.00		NIST Webbook
rinpol	3223.00		NIST Webbook
tb	1074.92	K	Joback Method
tc	1320.75	K	Joback Method
tf	640.93	K	Joback Method
vc	1.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1382.10	J/mol×K	1074.92	Joback Method
cpg	1398.30	J/mol×K	1115.89	Joback Method
cpg	1412.85	J/mol×K	1156.86	Joback Method
cpg	1425.83	J/mol×K	1197.84	Joback Method
cpg	1437.38	J/mol×K	1238.81	Joback Method
cpg	1447.58	J/mol×K	1279.78	Joback Method
cpg	1456.55	J/mol×K	1320.75	Joback Method
dvisc	0.0001582	Pa×s	640.93	Joback Method

dvisc	0.0000820	Pa×s	713.26	Joback Method
dvisc	0.0000480	Pa×s	785.59	Joback Method
dvisc	0.0000307	Pa×s	857.92	Joback Method
dvisc	0.0000211	Pa×s	930.26	Joback Method
dvisc	0.0000153	Pa×s	1002.59	Joback Method
dvisc	0.0000116	Pa×s	1074.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363708&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