

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:	NUQIMPDVRJHXB-T-UHFFFAOYSA-N
Formula:	C26H40O5
SMILES:	CCCCCCCCCCCCOC(=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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0000646	Paxs	755.31	Joback Method
dvisc	0.0000418	Paxs	823.77	Joback Method
dvisc	0.0000289	Paxs	892.24	Joback Method
dvisc	0.0000210	Paxs	960.70	Joback Method
dvisc	0.0000160	Paxs	1029.16	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363706&Units=SI

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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