

Dimethylmalonic acid, 4-acetylphenyl tetradecyl ester

Inchi:	InChI=1S/C27H42O5/c1-5-6-7-8-9-10-11-12-13-14-15-16-21-31-25(29)27(3,4)26(30)32-2
InchiKey:	AUPADCMNMPOLIE-UHFFFAOYSA-N
Formula:	C27H42O5
SMILES:	CCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1ccc(C(C)=O)cc1
Mol. weight [g/mol]:	446.62

Physical Properties

Property code	Value	Unit	Source
gf	-314.68	kJ/mol	Joback Method
hf	-986.48	kJ/mol	Joback Method
hfus	59.10	kJ/mol	Joback Method
hvap	102.40	kJ/mol	Joback Method
log10ws	-8.18		Crippen Method
logp	7.065		Crippen Method
mcvol	383.980	ml/mol	McGowan Method
pc	907.24	kPa	Joback Method
rinpol	3124.00		NIST Webbook
tb	1052.04	K	Joback Method
tc	1289.96	K	Joback Method
tf	629.66	K	Joback Method
vc	1.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1319.61	J/molxK	1052.04	Joback Method
cpg	1335.49	J/molxK	1091.69	Joback Method
cpg	1349.81	J/molxK	1131.35	Joback Method
cpg	1362.65	J/molxK	1171.00	Joback Method
cpg	1374.11	J/molxK	1210.65	Joback Method
cpg	1384.28	J/molxK	1250.31	Joback Method
cpg	1393.26	J/molxK	1289.96	Joback Method
dvisc	0.0001810	Paxs	629.66	Joback Method
dvisc	0.0000947	Paxs	700.06	Joback Method

dvisc	0.0000557	Paxs	770.45	Joback Method
dvisc	0.0000359	Paxs	840.85	Joback Method
dvisc	0.0000247	Paxs	911.25	Joback Method
dvisc	0.0000179	Paxs	981.64	Joback Method
dvisc	0.0000136	Paxs	1052.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363707&Units=SI
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

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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