Dimethylmalonic acid, 4-acetylphenyl undecyl ester

Inchi: InChI=1S/C24H36O5/c1-5-6-7-8-9-10-11-12-13-18-28-22(26)24(3,4)23(27)29-21-16-14-2

InchiKey: LLIAVONMTPUTQN-UHFFFAOYSA-N

Formula: C24H36O5

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

Mol. weight [g/mol]: 404.54

Physical Properties

Property code	Value	Unit	Source
gf	-339.94	kJ/mol	Joback Method
hf	-924.56	kJ/mol	Joback Method
hfus	51.33	kJ/mol	Joback Method
hvap	95.72	kJ/mol	Joback Method
log10ws	-6.93		Crippen Method
logp	5.895		Crippen Method
mcvol	341.710	ml/mol	McGowan Method
pc	1087.78	kPa	Joback Method
rinpol	2813.00		NIST Webbook
rinpol	2813.00		NIST Webbook
tb	983.40	K	Joback Method
tc	1204.63	K	Joback Method
tf	595.85	K	Joback Method
vc	1.315	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1134.49	J/mol×K	983.40	Joback Method
cpg	1149.62	J/mol×K	1020.27	Joback Method
cpg	1163.40	J/mol×K	1057.14	Joback Method
cpg	1175.89	J/mol×K	1094.02	Joback Method
cpg	1187.16	J/mol×K	1130.89	Joback Method
cpg	1197.27	J/mol×K	1167.76	Joback Method
cpg	1206.28	J/mol×K	1204.63	Joback Method
dvisc	0.0002672	Pa×s	595.85	Joback Method

dvisc	0.0001438	Pa×s	660.44	Joback Method
dvisc	0.0000864	Pa×s	725.03	Joback Method
dvisc	0.0000564	Pa×s	789.62	Joback Method
dvisc	0.0000393	Pa×s	854.22	Joback Method
dvisc	0.0000288	Pa×s	918.81	Joback Method
dvisc	0.0000220	Pa×s	983.40	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363705&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