Dimethylmalonic acid, 2-phenethyl undecyl ester

Inchi: InChI=1S/C24H38O4/c1-4-5-6-7-8-9-10-11-15-19-27-22(25)24(2,3)23(26)28-20-18-21-16
InchiKey: HVXYKRJBUCXRBD-UHFFFAOYSA-N
Formula: C24H38O4
SMILES: CCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCCc1ccccc1
Mol. weight [g/mol]: 390.56

Physical Properties

Property code	Value	Unit	Source
gf	-201.39	kJ/mol	Joback Method
hf	-800.51	kJ/mol	Joback Method
hfus	50.12	kJ/mol	Joback Method
hvap	88.31	kJ/mol	Joback Method
log10ws	-6.46		Crippen Method
logp	5.872		Crippen Method
mcvol	340.140	ml/mol	McGowan Method
pc	1054.14	kPa	Joback Method
rinpol	2616.00		NIST Webbook
tb	924.55	K	Joback Method
tc	1134.34	K	Joback Method
tf	533.40	K	Joback Method
vc	1.308	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1120.14	J/mol×K	924.55	Joback Method
cpg	1137.26	J/mol×K	959.51	Joback Method
cpg	1153.10	J/mol×K	994.48	Joback Method
cpg	1167.73	J/mol×K	1029.44	Joback Method
cpg	1181.20	J/mol×K	1064.41	Joback Method
cpg	1193.58	J/mol×K	1099.37	Joback Method
cpg	1204.94	J/mol×K	1134.34	Joback Method
dvisc	0.0003979	Pa×s	533.40	Joback Method
dvisc	0.0001915	Pa×s	598.59	Joback Method

dvisc	0.0001064	Pa×s	663.78	Joback Method
dvisc	0.0000657	Pa×s	728.97	Joback Method
dvisc	0.0000439	Pa×s	794.17	Joback Method
dvisc	0.0000312	Pa×s	859.36	Joback Method
dvisc	0.0000232	Pa×s	924.55	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=U361622&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