Dimethylmalonic acid, 2-phenethyl tridecyl ester

Inchi: InChI=1S/C26H42O4/c1-4-5-6-7-8-9-10-11-12-13-17-21-29-24(27)26(2,3)25(28)30-22-20

InchiKey: SVZWGOYYGHBITR-UHFFFAOYSA-N

Formula: C26H42O4

SMILES: CCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCCc1ccccc1

Mol. weight [g/mol]: 418.61

Physical Properties

Property code	Value	Unit	Source
gf	-184.55	kJ/mol	Joback Method
hf	-841.79	kJ/mol	Joback Method
hfus	55.30	kJ/mol	Joback Method
hvap	92.76	kJ/mol	Joback Method
log10ws	-7.29		Crippen Method
logp	6.653		Crippen Method
mcvol	368.320	ml/mol	McGowan Method
pc	934.06	kPa	Joback Method
rinpol	2811.00		NIST Webbook
tb	970.31	K	Joback Method
tc	1187.95	K	Joback Method
tf	555.94	K	Joback Method
vc	1.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1244.13	J/mol×K	970.31	Joback Method
cpg	1261.77	J/mol×K	1006.58	Joback Method
cpg	1278.02	J/mol×K	1042.86	Joback Method
cpg	1292.97	J/mol×K	1079.13	Joback Method
cpg	1306.69	J/mol×K	1115.41	Joback Method
cpg	1319.26	J/mol×K	1151.68	Joback Method
cpg	1330.75	J/mol×K	1187.95	Joback Method
dvisc	0.0003062	Pa×s	555.94	Joback Method
dvisc	0.0001448	Pa×s	625.00	Joback Method

dvisc	0.0000794	Pa×s	694.06	Joback Method
dvisc	0.0000486	Pa×s	763.12	Joback Method
dvisc	0.0000323	Pa×s	832.19	Joback Method
dvisc	0.0000228	Pa×s	901.25	Joback Method
dvisc	0.0000169	Pa×s	970.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361624&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
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