Dimethylmalonic acid, cis-4-methylcyclohexyl pentadecyl ester

Inchi: InChI=1S/C27H50O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-22-30-25(28)27(3,4)26(29)3

InchiKey: WWAIVOXWWCNTJR-UHFFFAOYSA-N

Formula: C27H50O4

SMILES: CCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OC1CCC(C)CC1

Mol. weight [g/mol]: 438.68

Physical Properties

Property code	Value	Unit	Source
gf	-271.80	kJ/mol	Joback Method
hf	-1064.98	kJ/mol	Joback Method
hfus	56.75	kJ/mol	Joback Method
hvap	92.83	kJ/mol	Joback Method
log10ws	-8.37		Crippen Method
logp	7.769		Crippen Method
mcvol	395.310	ml/mol	McGowan Method
pc	803.88	kPa	Joback Method
rinpol	2936.00		NIST Webbook
rinpol	2936.00		NIST Webbook
tb	981.39	K	Joback Method
tc	1202.04	K	Joback Method
tf	543.93	K	Joback Method
vc	1.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1410.07	J/mol×K	981.39	Joback Method
cpg	1430.28	J/mol×K	1018.16	Joback Method
cpg	1448.69	J/mol×K	1054.94	Joback Method
cpg	1465.38	J/mol×K	1091.71	Joback Method
cpg	1480.41	J/mol×K	1128.49	Joback Method
cpg	1493.87	J/mol×K	1165.26	Joback Method
cpg	1505.81	J/mol×K	1202.04	Joback Method
dvisc	0.0004012	Pa×s	543.93	Joback Method

dvisc	0.0001793	Pa×s	616.84	Joback Method
dvisc	0.0000950	Pa×s	689.75	Joback Method
dvisc	0.0000568	Pa×s	762.66	Joback Method
dvisc	0.0000372	Pa×s	835.57	Joback Method
dvisc	0.0000261	Pa×s	908.48	Joback Method
dvisc	0.0000192	Pa×s	981.39	Joback Method

Sources

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=U363888&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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