Dimethylmalonic acid, cis-4-methylcyclohexyl heptadecyl ester

Inchi: InChI=1S/C29H54O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-24-32-27(30)29(3,4)2

InchiKey: VGAFGWAKYAHZQB-UHFFFAOYSA-N

Formula: C29H54O4

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

Mol. weight [g/mol]: 466.74

Physical Properties

Property code	Value	Unit	Source
gf	-254.96	kJ/mol	Joback Method
hf	-1106.26	kJ/mol	Joback Method
hfus	61.93	kJ/mol	Joback Method
hvap	97.28	kJ/mol	Joback Method
log10ws	-9.21		Crippen Method
logp	8.549		Crippen Method
mcvol	423.490	ml/mol	McGowan Method
pc	723.02	kPa	Joback Method
rinpol	3155.00		NIST Webbook
rinpol	3155.00		NIST Webbook
tb	1027.15	K	Joback Method
tc	1262.54	K	Joback Method
tf	566.47	K	Joback Method
vc	1.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1539.28	J/mol×K	1027.15	Joback Method
cpg	1623.42	J/mol×K	1223.31	Joback Method
cpg	1610.29	J/mol×K	1184.08	Joback Method
cpg	1595.40	J/mol×K	1144.85	Joback Method
cpg	1578.67	J/mol×K	1105.61	Joback Method
cpg	1559.99	J/mol×K	1066.38	Joback Method
cpg	1634.89	J/mol×K	1262.54	Joback Method
dvisc	0.0000140	Pa×s	1027.15	Joback Method

dvisc	0.0000190	Pa×s	950.37	Joback Method
dvisc	0.0000272	Pa×s	873.59	Joback Method
dvisc	0.0000418	Pa×s	796.81	Joback Method
dvisc	0.0000703	Pa×s	720.03	Joback Method
dvisc	0.0001342	Pa×s	643.25	Joback Method
dvisc	0.0003048	Pa×s	566.47	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=U363890&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