Dimethylmalonic acid, cis-4-methylcyclohexyl hexadecyl ester

Inchi: InChI=1S/C28H52O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-23-31-26(29)28(3,4)27(3

InchiKey: FDWGPPHFZKPNCA-UHFFFAOYSA-N

Formula: C28H52O4

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

Mol. weight [g/mol]: 452.71

Physical Properties

Property code	Value	Unit	Source
gf	-263.38	kJ/mol	Joback Method
hf	-1085.62	kJ/mol	Joback Method
hfus	59.34	kJ/mol	Joback Method
hvap	95.06	kJ/mol	Joback Method
log10ws	-8.79		Crippen Method
logp	8.159		Crippen Method
mcvol	409.400	ml/mol	McGowan Method
pc	761.84	kPa	Joback Method
rinpol	3053.00		NIST Webbook
tb	1004.27	K	Joback Method
tc	1231.70	K	Joback Method
tf	555.20	K	Joback Method
vc	1.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1474.54	J/mol×K	1004.27	Joback Method
cpg	1558.48	J/mol×K	1193.79	Joback Method
cpg	1545.18	J/mol×K	1155.89	Joback Method
cpg	1530.22	J/mol×K	1117.98	Joback Method
cpg	1513.51	J/mol×K	1080.08	Joback Method
cpg	1494.98	J/mol×K	1042.17	Joback Method
cpg	1570.19	J/mol×K	1231.70	Joback Method
dvisc	0.0000164	Pa×s	1004.27	Joback Method
dvisc	0.0000222	Pa×s	929.42	Joback Method

dvisc	0.0000318	Pa×s	854.58	Joback Method
dvisc	0.0000488	Pa×s	779.74	Joback Method
dvisc	0.0000818	Pa×s	704.89	Joback Method
dvisc	0.0001553	Pa×s	630.05	Joback Method
dvisc	0.0003501	Pa×s	555.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363889&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

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