Dimethylmalonic acid, cis-4-methylcyclohexyl dodecyl ester

Inchi: InChI=1S/C24H44O4/c1-5-6-7-8-9-10-11-12-13-14-19-27-22(25)24(3,4)23(26)28-21-17-1

InchiKey: IFRYRCWHZHPKLC-UHFFFAOYSA-N

Formula: C24H44O4

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

Mol. weight [g/mol]: 396.60

Physical Properties

Property code	Value	Unit	Source
gf	-297.06	kJ/mol	Joback Method
hf	-1003.06	kJ/mol	Joback Method
hfus	48.98	kJ/mol	Joback Method
hvap	86.15	kJ/mol	Joback Method
log10ws	-7.12		Crippen Method
logp	6.599		Crippen Method
mcvol	353.040	ml/mol	McGowan Method
pc	953.19	kPa	Joback Method
rinpol	2640.00		NIST Webbook
tb	912.75	K	Joback Method
tc	1119.39	K	Joback Method
tf	510.12	K	Joback Method
vc	1.349	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1218.73	J/mol×K	912.75	Joback Method
cpg	1238.47	J/mol×K	947.19	Joback Method
cpg	1256.66	J/mol×K	981.63	Joback Method
cpg	1273.36	J/mol×K	1016.07	Joback Method
cpg	1288.61	J/mol×K	1050.51	Joback Method
cpg	1302.46	J/mol×K	1084.95	Joback Method
cpg	1314.96	J/mol×K	1119.39	Joback Method
dvisc	0.0005950	Pa×s	510.12	Joback Method
dvisc	0.0002727	Pa×s	577.23	Joback Method

dvisc	0.0001470	Pa×s	644.33	Joback Method
dvisc	0.0000891	Pa×s	711.43	Joback Method
dvisc	0.0000588	Pa×s	778.54	Joback Method
dvisc	0.0000415	Pa×s	845.64	Joback Method
dvisc	0.0000308	Pa×s	912.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363885&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