Dimethylmalonic acid, cis-4-methylcyclohexyl undecyl ester

Inchi: InChI=1S/C23H42O4/c1-5-6-7-8-9-10-11-12-13-18-26-21(24)23(3,4)22(25)27-20-16-14-1

InchiKey: VZVVSRJDZXMHRK-UHFFFAOYSA-N

Formula: C23H42O4

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

Mol. weight [g/mol]: 382.58

Physical Properties

Property code	Value	Unit	Source
gf	-305.48	kJ/mol	Joback Method
hf	-982.42	kJ/mol	Joback Method
hfus	46.39	kJ/mol	Joback Method
hvap	83.93	kJ/mol	Joback Method
log10ws	-6.70		Crippen Method
logp	6.209		Crippen Method
mcvol	338.950	ml/mol	McGowan Method
pc	1012.30	kPa	Joback Method
rinpol	2538.00		NIST Webbook
rinpol	2538.00		NIST Webbook
tb	889.87	K	Joback Method
tc	1093.71	K	Joback Method
tf	498.85	K	Joback Method
vc	1.292	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1155.80	J/mol×K	889.87	Joback Method
cpg	1175.45	J/mol×K	923.84	Joback Method
cpg	1193.61	J/mol×K	957.82	Joback Method
cpg	1210.33	J/mol×K	991.79	Joback Method
cpg	1225.65	J/mol×K	1025.76	Joback Method
cpg	1239.62	J/mol×K	1059.74	Joback Method
cpg	1252.28	J/mol×K	1093.71	Joback Method
dvisc	0.0006748	Pa×s	498.85	Joback Method

dvisc	0.0003120	Pa×s	564.02	Joback Method
dvisc	0.0001693	Pa×s	629.19	Joback Method
dvisc	0.0001030	Pa×s	694.36	Joback Method
dvisc	0.0000683	Pa×s	759.53	Joback Method
dvisc	0.0000483	Pa×s	824.70	Joback Method
dvisc	0.0000359	Pa×s	889.87	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=U363884&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

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