Dimethylmalonic acid, cis-4-methylcyclohexyl tridecyl ester

Inchi: InChI=1S/C25H46O4/c1-5-6-7-8-9-10-11-12-13-14-15-20-28-23(26)25(3,4)24(27)29-22-1

InchiKey: PWQUAZPRRYIBNE-UHFFFAOYSA-N

Formula: C25H46O4

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

Mol. weight [g/mol]: 410.63

Physical Properties

Property code	Value	Unit	Source
gf	-288.64	kJ/mol	Joback Method
hf	-1023.70	kJ/mol	Joback Method
hfus	51.57	kJ/mol	Joback Method
hvap	88.38	kJ/mol	Joback Method
log10ws	-7.54		Crippen Method
logp	6.989		Crippen Method
mcvol	367.130	ml/mol	McGowan Method
pc	899.10	kPa	Joback Method
rinpol	2742.00		NIST Webbook
rinpol	2742.00		NIST Webbook
tb	935.63	K	Joback Method
tc	1145.96	K	Joback Method
tf	521.39	K	Joback Method
vc	1.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1282.12	J/mol×K	935.63	Joback Method
cpg	1365.81	J/mol×K	1110.90	Joback Method
cpg	1352.08	J/mol×K	1075.85	Joback Method
cpg	1336.90	J/mol×K	1040.79	Joback Method
cpg	1320.22	J/mol×K	1005.74	Joback Method
cpg	1301.98	J/mol×K	970.68	Joback Method
cpg	1378.14	J/mol×K	1145.96	Joback Method
dvisc	0.0000264	Pa×s	935.63	Joback Method

dvisc	0.0000356	Pa×s	866.59	Joback Method
dvisc	0.0000506	Pa×s	797.55	Joback Method
dvisc	0.0000768	Pa×s	728.51	Joback Method
dvisc	0.0001274	Pa×s	659.47	Joback Method
dvisc	0.0002376	Pa×s	590.43	Joback Method
dvisc	0.0005231	Pa×s	521.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363886&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

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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