Dimethylmalonic acid, decyl trans-4-methylcyclohexyl ester

Inchi: InChI=1S/C22H40O4/c1-5-6-7-8-9-10-11-12-17-25-20(23)22(3,4)21(24)26-19-15-13-18(2

InchiKey: FLRGZQGFCSBNAF-UHFFFAOYSA-N

Formula: C22H40O4

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

Mol. weight [g/mol]: 368.55

Physical Properties

Property code	Value	Unit	Source
gf	-313.90	kJ/mol	Joback Method
hf	-961.78	kJ/mol	Joback Method
hfus	43.80	kJ/mol	Joback Method
hvap	81.70	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	5.818		Crippen Method
mcvol	324.860	ml/mol	McGowan Method
pc	1077.10	kPa	Joback Method
rinpol	2407.00		NIST Webbook
rinpol	2407.00		NIST Webbook
tb	866.99	K	Joback Method
tc	1068.86	K	Joback Method
tf	487.58	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1093.39	J/mol×K	866.99	Joback Method
cpg	1112.97	J/mol×K	900.63	Joback Method
cpg	1131.12	J/mol×K	934.28	Joback Method
cpg	1147.87	J/mol×K	967.92	Joback Method
cpg	1163.26	J/mol×K	1001.57	Joback Method
cpg	1177.33	J/mol×K	1035.21	Joback Method
cpg	1190.13	J/mol×K	1068.86	Joback Method
dvisc	0.0007630	Pa×s	487.58	Joback Method

dvisc	0.0003562	Pa×s	550.81	Joback Method
dvisc	0.0001945	Pa×s	614.05	Joback Method
dvisc	0.0001189	Pa×s	677.28	Joback Method
dvisc	0.0000791	Pa×s	740.52	Joback Method
dvisc	0.0000561	Pa×s	803.75	Joback Method
dvisc	0.0000418	Pa×s	866.99	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=U363902&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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