Dimethylmalonic acid, neopentyl tridecyl ester

Inchi: InChI=1S/C23H44O4/c1-7-8-9-10-11-12-13-14-15-16-17-18-26-20(24)23(5,6)21(25)27-1
InchiKey: ZBFHKRIKCIDNHZ-UHFFFAOYSA-N
Formula: C23H44O4
SMILES: CCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCC(C)(C)C
Mol. weight [g/mol]: 384.59

Physical Properties

Property code	Value	Unit	Source
gf	-319.38	kJ/mol	Joback Method
hf	-1025.15	kJ/mol	Joback Method
hfus	46.07	kJ/mol	Joback Method
hvap	82.51	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	6.456		Crippen Method
mcvol	349.810	ml/mol	McGowan Method
pc	920.50	kPa	Joback Method
rinpol	2334.00		NIST Webbook
tb	871.76	K	Joback Method
tc	1068.39	K	Joback Method
tf	498.13	K	Joback Method
vc	1.349	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1155.11	J/mol×K	871.76	Joback Method
cpg	1174.37	J/mol×K	904.53	Joback Method
cpg	1192.44	J/mol×K	937.30	Joback Method
cpg	1209.37	J/mol×K	970.08	Joback Method
cpg	1225.23	J/mol×K	1002.85	Joback Method
cpg	1240.07	J/mol×K	1035.62	Joback Method
cpg	1253.96	J/mol×K	1068.39	Joback Method
dvisc	0.0005037	Pa×s	498.13	Joback Method
dvisc	0.0002210	Pa×s	560.40	Joback Method

dvisc	0.0001143	Pa×s	622.67	Joback Method
dvisc	0.0000667	Pa×s	684.94	Joback Method
dvisc	0.0000425	Pa×s	747.22	Joback Method
dvisc	0.0000291	Pa×s	809.49	Joback Method
dvisc	0.0000210	Pa×s	871.76	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=U361753&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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