

Dimethylmalonic acid, dodecyl hexyl ester

Inchi:	InChI=1S/C23H44O4/c1-5-7-9-11-12-13-14-15-16-18-20-27-22(25)23(3,4)21(24)26-19-1
InchiKey:	WKEGSDVADKCCCTE-UHFFFAOYSA-N
Formula:	C23H44O4
SMILES:	CCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCCCCC
Mol. weight [g/mol]:	384.59

Physical Properties

Property code	Value	Unit	Source
gf	-322.22	kJ/mol	Joback Method
hf	-1016.40	kJ/mol	Joback Method
hfus	53.49	kJ/mol	Joback Method
hvap	83.81	kJ/mol	Joback Method
log10ws	-6.93		Crippen Method
logp	6.600		Crippen Method
mvol	349.810	ml/mol	McGowan Method
pc	909.98	kPa	Joback Method
rinpol	2417.00		NIST Webbook
rinpol	2417.00		NIST Webbook
tb	874.99	K	Joback Method
tc	1071.31	K	Joback Method
tf	495.71	K	Joback Method
vc	1.361	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1154.79	J/molxK	874.99	Joback Method
cpg	1174.20	J/molxK	907.71	Joback Method
cpg	1192.37	J/molxK	940.43	Joback Method
cpg	1209.35	J/molxK	973.15	Joback Method
cpg	1225.18	J/molxK	1005.87	Joback Method
cpg	1239.91	J/molxK	1038.59	Joback Method
cpg	1253.57	J/molxK	1071.31	Joback Method
dvisc	0.0005484	Paxs	495.71	Joback Method

dvisc	0.0002494	Paxs	558.92	Joback Method
dvisc	0.0001331	Paxs	622.14	Joback Method
dvisc	0.0000798	Paxs	685.35	Joback Method
dvisc	0.0000521	Paxs	748.56	Joback Method
dvisc	0.0000364	Paxs	811.78	Joback Method
dvisc	0.0000268	Paxs	874.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361693&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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