

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:	CCCCCCCCCCCCOC(=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/molxK	871.76	Joback Method
cpg	1174.37	J/molxK	904.53	Joback Method
cpg	1192.44	J/molxK	937.30	Joback Method
cpg	1209.37	J/molxK	970.08	Joback Method
cpg	1225.23	J/molxK	1002.85	Joback Method
cpg	1240.07	J/molxK	1035.62	Joback Method
cpg	1253.96	J/molxK	1068.39	Joback Method
dvisc	0.0005037	Paxs	498.13	Joback Method
dvisc	0.0002210	Paxs	560.40	Joback Method

dvisc	0.0001143	Paxs	622.67	Joback Method
dvisc	0.0000667	Paxs	684.94	Joback Method
dvisc	0.0000425	Paxs	747.22	Joback Method
dvisc	0.0000291	Paxs	809.49	Joback Method
dvisc	0.0000210	Paxs	871.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361753&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

Latest version available from:

<https://www.chemeo.com/cid/53-384-7/Dimethylmalonic-acid-neopentyl-tridecyl-ester.pdf>

Generated by Cheméo on 2024-04-24 01:31:38.763897266 +0000 UTC m=+16211547.684474583.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.