

Dimethylmalonic acid, heptadecyl neopentyl ester

Inchi: InChI=1S/C27H52O4/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-30-24(28)27(5,
InchiKey: ILVDDEOEDNKTGJ-UHFFFAOYSA-N
Formula: C27H52O4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCC(C)(C)C
Mol. weight [g/mol]: 440.70

Physical Properties

Property code	Value	Unit	Source
gf	-285.70	kJ/mol	Joback Method
hf	-1107.71	kJ/mol	Joback Method
hfus	56.43	kJ/mol	Joback Method
hvap	91.42	kJ/mol	Joback Method
log10ws	-8.37		Crippen Method
logp	8.017		Crippen Method
mcvol	406.170	ml/mol	McGowan Method
pc	738.42	kPa	Joback Method
rinpol	2725.00		NIST Webbook
tb	963.28	K	Joback Method
tc	1182.44	K	Joback Method
tf	543.21	K	Joback Method
vc	1.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1408.99	J/molxK	963.28	Joback Method
cpg	1430.15	J/molxK	999.81	Joback Method
cpg	1449.83	J/molxK	1036.33	Joback Method
cpg	1468.14	J/molxK	1072.86	Joback Method
cpg	1485.18	J/molxK	1109.39	Joback Method
cpg	1501.02	J/molxK	1145.91	Joback Method
cpg	1515.79	J/molxK	1182.44	Joback Method
dvisc	0.0002815	Paxs	543.21	Joback Method
dvisc	0.0001197	Paxs	613.22	Joback Method

dvisc	0.0000606	Paxs	683.23	Joback Method
dvisc	0.0000348	Paxs	753.25	Joback Method
dvisc	0.0000220	Paxs	823.26	Joback Method
dvisc	0.0000149	Paxs	893.27	Joback Method
dvisc	0.0000107	Paxs	963.28	Joback Method

Sources

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=U361757&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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