

Dimethylmalonic acid, hexadecyl neopentyl ester

Inchi:	InChI=1S/C26H50O4/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-29-23(27)26(5,6)2
InchiKey:	VHHAQPBAKCRDLI-UHFFFAOYSA-N
Formula:	C26H50O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCC(C)(C)C
Mol. weight [g/mol]:	426.67

Physical Properties

Property code	Value	Unit	Source
gf	-294.12	kJ/mol	Joback Method
hf	-1087.07	kJ/mol	Joback Method
hfus	53.84	kJ/mol	Joback Method
hvap	89.19	kJ/mol	Joback Method
log10ws	-7.95		Crippen Method
logp	7.626		Crippen Method
mcvol	392.080	ml/mol	McGowan Method
pc	778.51	kPa	Joback Method
rinsol	2633.00		NIST Webbook
tb	940.40	K	Joback Method
tc	1152.38	K	Joback Method
tf	531.94	K	Joback Method
vc	1.518	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1344.74	J/molxK	940.40	Joback Method
cpg	1434.68	J/molxK	1117.05	Joback Method
cpg	1419.13	J/molxK	1081.72	Joback Method
cpg	1402.44	J/molxK	1046.39	Joback Method
cpg	1384.53	J/molxK	1011.06	Joback Method
cpg	1365.33	J/molxK	975.73	Joback Method
cpg	1449.18	J/molxK	1152.38	Joback Method
dvisc	0.0000127	Paxs	940.40	Joback Method
dvisc	0.0000177	Paxs	872.32	Joback Method

dvisc	0.0000260	Paxs	804.25	Joback Method
dvisc	0.0000411	Paxs	736.17	Joback Method
dvisc	0.0000712	Paxs	668.09	Joback Method
dvisc	0.0001398	Paxs	600.02	Joback Method
dvisc	0.0003265	Paxs	531.94	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361756&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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