

Dimethylmalonic acid, 2-naphthylmethyl octyl ester

Inchi:	InChI=1S/C24H32O4/c1-4-5-6-7-8-11-16-27-22(25)24(2,3)23(26)28-18-19-14-15-20-12-9
InchiKey:	FYJIJNLOGIVGHU-UHFFFAOYSA-N
Formula:	C24H32O4
SMILES:	CCCCCCCCOC(=O)C(C)(C)C(=O)OCc1ccc2ccccc2c1
Mol. weight [g/mol]:	384.51

Physical Properties

Property code	Value	Unit	Source
gf	-104.37	kJ/mol	Joback Method
hf	-620.91	kJ/mol	Joback Method
hfus	46.75	kJ/mol	Joback Method
hvap	90.61	kJ/mol	Joback Method
log10ws	-7.08		Crippen Method
logp	5.813		Crippen Method
mcvol	320.680	ml/mol	McGowan Method
pc	1231.15	kPa	Joback Method
rinpol	2842.00		NIST Webbook
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tb	948.51	K	Joback Method
tc	1168.74	K	Joback Method
tf	578.62	K	Joback Method
vc	1.230	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1040.19	J/molxK	948.51	Joback Method
cpg	1107.77	J/molxK	1132.04	Joback Method
cpg	1096.09	J/molxK	1095.33	Joback Method
cpg	1083.59	J/molxK	1058.63	Joback Method
cpg	1070.16	J/molxK	1021.92	Joback Method
cpg	1055.73	J/molxK	985.22	Joback Method
cpg	1118.70	J/molxK	1168.74	Joback Method
dvisc	0.0000485	Paxs	948.51	Joback Method

dvisc	0.0000614	Paxs	886.86	Joback Method
dvisc	0.0000806	Paxs	825.21	Joback Method
dvisc	0.0001106	Paxs	763.57	Joback Method
dvisc	0.0001605	Paxs	701.92	Joback Method
dvisc	0.0002500	Paxs	640.27	Joback Method
dvisc	0.0004280	Paxs	578.62	Joback Method

Sources

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=U363861&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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