

Dimethylmalonic acid, 2-naphthylmethyl propyl ester

Inchi:	InChI=1S/C19H22O4/c1-4-11-22-17(20)19(2,3)18(21)23-13-14-9-10-15-7-5-6-8-16(15)12
InchiKey:	XMMQASJHRMLRBX-UHFFFAOYSA-N
Formula:	C19H22O4
SMILES:	CCCOC(=O)C(C)(C)C(=O)OCc1ccc2ccccc2c1
Mol. weight [g/mol]:	314.38

Physical Properties

Property code	Value	Unit	Source
gf	-146.47	kJ/mol	Joback Method
hf	-517.71	kJ/mol	Joback Method
hfus	33.80	kJ/mol	Joback Method
hvap	79.48	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	3.862		Crippen Method
mcvol	250.230	ml/mol	McGowan Method
pc	1780.34	kPa	Joback Method
rinpol	2366.00		NIST Webbook
rinpol	2366.00		NIST Webbook
tb	834.11	K	Joback Method
tc	1057.24	K	Joback Method
tf	522.27	K	Joback Method
vc	0.951	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	746.82	J/molxK	834.11	Joback Method
cpg	761.35	J/molxK	871.30	Joback Method
cpg	774.80	J/molxK	908.49	Joback Method
cpg	787.23	J/molxK	945.67	Joback Method
cpg	798.71	J/molxK	982.86	Joback Method
cpg	809.34	J/molxK	1020.05	Joback Method
cpg	819.17	J/molxK	1057.24	Joback Method
dvisc	0.0007020	Paxs	522.27	Joback Method

dvisc	0.0004351	Paxs	574.24	Joback Method
dvisc	0.0002919	Paxs	626.22	Joback Method
dvisc	0.0002082	Paxs	678.19	Joback Method
dvisc	0.0001558	Paxs	730.16	Joback Method
dvisc	0.0001212	Paxs	782.14	Joback Method
dvisc	0.0000973	Paxs	834.11	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=U363856&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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