

Dimethylmalonic acid, heptyl 2-naphthylmethyl ester

Inchi:	InChI=1S/C23H30O4/c1-4-5-6-7-10-15-26-21(24)23(2,3)22(25)27-17-18-13-14-19-11-8-9
InchiKey:	OBISYGFZWIQBED-UHFFFAOYSA-N
Formula:	C23H30O4
SMILES:	CCCCCCCOC(=O)C(C)(C)C(=O)OCc1ccc2ccccc2c1
Mol. weight [g/mol]:	370.48

Physical Properties

Property code	Value	Unit	Source
gf	-112.79	kJ/mol	Joback Method
hf	-600.27	kJ/mol	Joback Method
hfus	44.16	kJ/mol	Joback Method
hvap	88.39	kJ/mol	Joback Method
log10ws	-6.66		Crippen Method
logp	5.423		Crippen Method
mcvol	306.590	ml/mol	McGowan Method
pc	1318.48	kPa	Joback Method
rinpol	2748.00		NIST Webbook
tb	925.63	K	Joback Method
tc	1144.91	K	Joback Method
tf	567.35	K	Joback Method
vc	1.175	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	980.06	J/molxK	925.63	Joback Method
cpg	995.38	J/molxK	962.18	Joback Method
cpg	1009.60	J/molxK	998.72	Joback Method
cpg	1022.82	J/molxK	1035.27	Joback Method
cpg	1035.11	J/molxK	1071.82	Joback Method
cpg	1046.57	J/molxK	1108.37	Joback Method
cpg	1057.28	J/molxK	1144.91	Joback Method
dvisc	0.0004763	Paxs	567.35	Joback Method
dvisc	0.0002813	Paxs	627.06	Joback Method

dvisc	0.0001820	Paxs	686.78	Joback Method
dvisc	0.0001263	Paxs	746.49	Joback Method
dvisc	0.0000925	Paxs	806.20	Joback Method
dvisc	0.0000707	Paxs	865.92	Joback Method
dvisc	0.0000560	Paxs	925.63	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=U363860&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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