

Diethylmalonic acid, 1-naphthyl pentyl ester

Inchi:	InChI=1S/C22H28O4/c1-4-7-10-16-25-20(23)22(5-2,6-3)21(24)26-19-15-11-13-17-12-8-9
InchiKey:	HEHCRBYIGPISEZ-UHFFFAOYSA-N
Formula:	C22H28O4
SMILES:	CCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc2ccccc12
Mol. weight [g/mol]:	356.46

Physical Properties

Property code	Value	Unit	Source
gf	-121.21	kJ/mol	Joback Method
hf	-579.63	kJ/mol	Joback Method
hfus	41.57	kJ/mol	Joback Method
hvap	86.16	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	5.285		Crippen Method
mcvol	292.500	ml/mol	McGowan Method
pc	1415.44	kPa	Joback Method
rinpol	2530.00		NIST Webbook
tb	902.75	K	Joback Method
tc	1121.90	K	Joback Method
tf	556.08	K	Joback Method
vc	1.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	920.61	J/molxK	902.75	Joback Method
cpg	935.72	J/molxK	939.27	Joback Method
cpg	949.75	J/molxK	975.80	Joback Method
cpg	962.77	J/molxK	1012.32	Joback Method
cpg	974.87	J/molxK	1048.85	Joback Method
cpg	986.12	J/molxK	1085.37	Joback Method
cpg	996.61	J/molxK	1121.90	Joback Method
dvisc	0.0005280	Paxs	556.08	Joback Method
dvisc	0.0003154	Paxs	613.86	Joback Method

dvisc	0.0002059	Paxs	671.64	Joback Method
dvisc	0.0001438	Paxs	729.41	Joback Method
dvisc	0.0001059	Paxs	787.19	Joback Method
dvisc	0.0000813	Paxs	844.97	Joback Method
dvisc	0.0000645	Paxs	902.75	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=U369869&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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