

Diethylmalonic acid, di(1-naphthyl) ester

Inchi:	InChI=1S/C27H24O4/c1-3-27(4-2,25(28)30-23-17-9-13-19-11-5-7-15-21(19)23)26(29)31
InchiKey:	QZQGMTCLCSTFQW-UHFFFAOYSA-N
Formula:	C27H24O4
SMILES:	CCC(CC)(C(=O)Oc1cccc2ccccc12)C(=O)Oc1cccc2ccccc12
Mol. weight [g/mol]:	412.48

Physical Properties

Property code	Value	Unit	Source
gf	130.32	kJ/mol	Joback Method
hf	-266.70	kJ/mol	Joback Method
hfus	45.19	kJ/mol	Joback Method
hvap	101.87	kJ/mol	Joback Method
log10ws	-8.37		Crippen Method
logp	6.310		Crippen Method
mcvol	319.730	ml/mol	McGowan Method
pc	1505.81	kPa	Joback Method
rinsol	3351.00		NIST Webbook
tb	1067.79	K	Joback Method
tc	1323.35	K	Joback Method
tf	684.07	K	Joback Method
vc	1.212	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1027.42	J/molxK	1067.79	Joback Method
cpg	1040.98	J/molxK	1110.38	Joback Method
cpg	1053.94	J/molxK	1152.98	Joback Method
cpg	1066.48	J/molxK	1195.57	Joback Method
cpg	1078.80	J/molxK	1238.16	Joback Method
cpg	1091.10	J/molxK	1280.75	Joback Method
cpg	1103.56	J/molxK	1323.35	Joback Method
dvisc	0.0003858	Paxs	684.07	Joback Method
dvisc	0.0002586	Paxs	748.02	Joback Method

dvisc	0.0001847	Paxs	811.98	Joback Method
dvisc	0.0001385	Paxs	875.93	Joback Method
dvisc	0.0001080	Paxs	939.88	Joback Method
dvisc	0.0000870	Paxs	1003.84	Joback Method
dvisc	0.0000719	Paxs	1067.79	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=U369876&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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