

Diethylmalonic acid, 1-naphthyl nonyl ester

Inchi:	InChI=1S/C26H36O4/c1-4-7-8-9-10-11-14-20-29-24(27)26(5-2,6-3)25(28)30-23-19-15-17
InchiKey:	RPAKTAZNXWILDK-UHFFFAOYSA-N
Formula:	C26H36O4
SMILES:	CCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc2ccccc12
Mol. weight [g/mol]:	412.56

Physical Properties

Property code	Value	Unit	Source
gf	-87.53	kJ/mol	Joback Method
hf	-662.19	kJ/mol	Joback Method
hfus	51.93	kJ/mol	Joback Method
hvap	95.06	kJ/mol	Joback Method
log10ws	-8.07		Crippen Method
logp	6.845		Crippen Method
mcvol	348.860	ml/mol	McGowan Method
pc	1080.64	kPa	Joback Method
rinpol	2911.00		NIST Webbook
tb	994.27	K	Joback Method
tc	1219.05	K	Joback Method
tf	601.16	K	Joback Method
vc	1.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1162.32	J/molxK	994.27	Joback Method
cpg	1178.38	J/molxK	1031.73	Joback Method
cpg	1193.32	J/molxK	1069.20	Joback Method
cpg	1207.24	J/molxK	1106.66	Joback Method
cpg	1220.24	J/molxK	1144.12	Joback Method
cpg	1232.42	J/molxK	1181.59	Joback Method
cpg	1243.88	J/molxK	1219.05	Joback Method
dvisc	0.0003422	Paxs	601.16	Joback Method
dvisc	0.0001956	Paxs	666.68	Joback Method

dvisc	0.0001236	Paxs	732.20	Joback Method
dvisc	0.0000842	Paxs	797.72	Joback Method
dvisc	0.0000608	Paxs	863.23	Joback Method
dvisc	0.0000460	Paxs	928.75	Joback Method
dvisc	0.0000361	Paxs	994.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369873&Units=SI
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

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
mccvol:	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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