

Diethylmalonic acid, decyl 2-naphthyl ester

Inchi:

InChI=1S/C27H38O4/c1-4-7-8-9-10-11-12-15-20-30-25(28)27(5-2,6-3)26(29)31-24-19-18

InchiKey:

XOBVPXJYOCADHF-UHFFFAOYSA-N

Formula:

C27H38O4

SMILES:

CCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc2ccccc2c1

Mol. weight [g/mol]:

426.59

Physical Properties

Property code	Value	Unit	Source
gf	-79.11	kJ/mol	Joback Method
hf	-682.83	kJ/mol	Joback Method
hfus	54.52	kJ/mol	Joback Method
hvap	97.29	kJ/mol	Joback Method
log10ws	-8.49		Crippen Method
logp	7.235		Crippen Method
mcvol	362.950	ml/mol	McGowan Method
pc	1015.53	kPa	Joback Method
rinpol	3084.00		NIST Webbook
tb	1017.15	K	Joback Method
tc	1245.65	K	Joback Method
tf	612.43	K	Joback Method
vc	1.399	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1224.23	J/molxK	1017.15	Joback Method
cpg	1240.62	J/molxK	1055.23	Joback Method
cpg	1255.87	J/molxK	1093.32	Joback Method
cpg	1270.09	J/molxK	1131.40	Joback Method
cpg	1283.39	J/molxK	1169.49	Joback Method
cpg	1295.87	J/molxK	1207.57	Joback Method
cpg	1307.66	J/molxK	1245.65	Joback Method
dvisc	0.0003046	Paxs	612.43	Joback Method
dvisc	0.0001724	Paxs	679.88	Joback Method

dvisc	0.0001081	Paxs	747.34	Joback Method
dvisc	0.0000732	Paxs	814.79	Joback Method
dvisc	0.0000527	Paxs	882.24	Joback Method
dvisc	0.0000397	Paxs	949.70	Joback Method
dvisc	0.0000310	Paxs	1017.15	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U369888&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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