

Diethylmalonic acid, 2-naphthyl propyl ester

Inchi:

InChI=1S/C20H24O4/c1-4-13-23-18(21)20(5-2,6-3)19(22)24-17-12-11-15-9-7-8-10-16(15)

InchiKey:

IKDPZXQXOKOVRW-UHFFFAOYSA-N

Formula:

C20H24O4

SMILES:

CCCOC(=O)C(CC)(CC)C(=O)Oc1ccc2ccccc2c1

Mol. weight [g/mol]:

328.40

Physical Properties

Property code	Value	Unit	Source
gf	-138.05	kJ/mol	Joback Method
hf	-538.35	kJ/mol	Joback Method
hfus	36.39	kJ/mol	Joback Method
hvap	81.71	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	4.505		Crippen Method
mcvol	264.320	ml/mol	McGowan Method
pc	1644.42	kPa	Joback Method
rinpol	2407.00		NIST Webbook
rinpol	2407.00		NIST Webbook
tb	856.99	K	Joback Method
tc	1078.11	K	Joback Method
tf	533.54	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	803.94	J/mol×K	856.99	Joback Method
cpg	867.50	J/mol×K	1041.25	Joback Method
cpg	856.66	J/mol×K	1004.40	Joback Method
cpg	844.95	J/mol×K	967.55	Joback Method
cpg	832.32	J/mol×K	930.70	Joback Method
cpg	818.67	J/mol×K	893.84	Joback Method
cpg	877.56	J/mol×K	1078.11	Joback Method
dvisc	0.0000851	Pa×s	856.99	Joback Method

dvisc	0.0001064	Pa×s	803.08	Joback Method
dvisc	0.0001374	Pa×s	749.17	Joback Method
dvisc	0.0001847	Pa×s	695.26	Joback Method
dvisc	0.0002608	Pa×s	641.36	Joback Method
dvisc	0.0003924	Pa×s	587.45	Joback Method
dvisc	0.0006413	Pa×s	533.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369880&Units=SI
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

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log_{10ws}:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
p_c:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/16-693-5/Diethylmalonic-acid-2-naphthyl-propyl-ester.pdf>

Generated by Cheméo on 2025-12-05 21:31:50.738774888 +0000 UTC m=+4718508.268815543.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.