

Diethylmalonic acid, 2-naphthyl octyl ester

Inchi:	InChI=1S/C25H34O4/c1-4-7-8-9-10-13-18-28-23(26)25(5-2,6-3)24(27)29-22-17-16-20-14
InchiKey:	SSNNGFMNQKLFSN-UHFFFAOYSA-N
Formula:	C25H34O4
SMILES:	CCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc2ccccc2c1
Mol. weight [g/mol]:	398.54

Physical Properties

Property code	Value	Unit	Source
gf	-95.95	kJ/mol	Joback Method
hf	-641.55	kJ/mol	Joback Method
hfus	49.34	kJ/mol	Joback Method
hvap	92.84	kJ/mol	Joback Method
log10ws	-7.65		Crippen Method
logp	6.455		Crippen Method
mcvol	334.770	ml/mol	McGowan Method
pc	1152.22	kPa	Joback Method
rinsol	2871.00		NIST Webbook
tb	971.39	K	Joback Method
tc	1193.44	K	Joback Method
tf	589.89	K	Joback Method
vc	1.286	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1100.96	J/molxK	971.39	Joback Method
cpg	1116.74	J/molxK	1008.40	Joback Method
cpg	1131.41	J/molxK	1045.41	Joback Method
cpg	1145.07	J/molxK	1082.41	Joback Method
cpg	1157.80	J/molxK	1119.42	Joback Method
cpg	1169.72	J/molxK	1156.43	Joback Method
cpg	1180.90	J/molxK	1193.44	Joback Method
dvisc	0.0003833	Paxs	589.89	Joback Method
dvisc	0.0002215	Paxs	653.47	Joback Method

dvisc	0.0001410	Paxs	717.06	Joback Method
dvisc	0.0000967	Paxs	780.64	Joback Method
dvisc	0.0000701	Paxs	844.22	Joback Method
dvisc	0.0000532	Paxs	907.81	Joback Method
dvisc	0.0000419	Paxs	971.39	Joback Method

Sources

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=U369886&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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