

Diethylmalonic acid, butyl 2-naphthyl ester

Inchi:	InChI=1S/C21H26O4/c1-4-7-14-24-19(22)21(5-2,6-3)20(23)25-18-13-12-16-10-8-9-11-17
InchiKey:	WRRBJIAEAOXHJ-UHFFFAOYSA-N
Formula:	C21H26O4
SMILES:	CCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc2ccccc2c1
Mol. weight [g/mol]:	342.43

Physical Properties

Property code	Value	Unit	Source
gf	-129.63	kJ/mol	Joback Method
hf	-558.99	kJ/mol	Joback Method
hfus	38.98	kJ/mol	Joback Method
hvap	83.93	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	4.895		Crippen Method
mcvol	278.410	ml/mol	McGowan Method
pc	1523.50	kPa	Joback Method
rinpol	2497.00		NIST Webbook
rinpol	2497.00		NIST Webbook
tb	879.87	K	Joback Method
tc	1099.65	K	Joback Method
tf	544.81	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	861.88	J/molxK	879.87	Joback Method
cpg	926.43	J/molxK	1063.02	Joback Method
cpg	915.38	J/molxK	1026.39	Joback Method
cpg	903.48	J/molxK	989.76	Joback Method
cpg	890.65	J/molxK	953.13	Joback Method
cpg	876.81	J/molxK	916.50	Joback Method
cpg	936.71	J/molxK	1099.65	Joback Method
dvisc	0.0000742	Paxs	879.87	Joback Method

dvisc	0.0000931	Paxs	824.03	Joback Method
dvisc	0.0001208	Paxs	768.18	Joback Method
dvisc	0.0001632	Paxs	712.34	Joback Method
dvisc	0.0002321	Paxs	656.50	Joback Method
dvisc	0.0003525	Paxs	600.65	Joback Method
dvisc	0.0005831	Paxs	544.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369882&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

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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