Diethylmalonic acid, butyl 1-naphthyl ester

Inchi: InChI=1S/C21H26O4/c1-4-7-15-24-19(22)21(5-2,6-3)20(23)25-18-14-10-12-16-11-8-9-13
InchiKey: TXVQCESZNIZRCU-UHFFFAOYSA-N
Formula: C21H26O4
SMILES: CCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc2ccccc12
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	2439.00		NIST Webbook
rinpol	2439.00		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/mol×K	879.87	Joback Method
cpg	876.81	J/mol×K	916.50	Joback Method
cpg	890.65	J/mol×K	953.13	Joback Method
cpg	903.48	J/mol×K	989.76	Joback Method
cpg	915.38	J/mol×K	1026.39	Joback Method
cpg	926.43	J/mol×K	1063.02	Joback Method
cpg	936.71	J/mol×K	1099.65	Joback Method
dvisc	0.0005831	Pa×s	544.81	Joback Method

dvisc	0.0003525	Pa×s	600.65	Joback Method
dvisc	0.0002321	Pa×s	656.50	Joback Method
dvisc	0.0001632	Pa×s	712.34	Joback Method
dvisc	0.0001208	Pa×s	768.18	Joback Method
dvisc	0.0000931	Pa×s	824.03	Joback Method
dvisc	0.0000742	Pa×s	879.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369868&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

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