Diethylmalonic acid, hexyl 2-naphthyl ester

Inchi: InChI=1S/C23H30O4/c1-4-7-8-11-16-26-21(24)23(5-2,6-3)22(25)27-20-15-14-18-12-9-10
InchiKey: PLZUOACTSSPGHJ-UHFFFAOYSA-N
Formula: C23H30O4
SMILES: CCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc2ccccc2c1
Mol. weight [g/mol]: 370.48

Physical Properties

Property code	Value	Unit	Source
gf	-112.79	kJ/mol	Joback Method
hf	-600.27	kJ/mol	Joback Method
hfus	44.16	kJ/mol	Joback Method
hvap	88.39	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	5.675		Crippen Method
mcvol	306.590	ml/mol	McGowan Method
pc	1318.48	kPa	Joback Method
rinpol	2680.00		NIST Webbook
tb	925.63	K	Joback Method
tc	1144.91	K	Joback Method
tf	567.35	K	Joback Method
vc	1.175	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	980.06	J/mol×K	925.63	Joback Method
cpg	995.38	J/mol×K	962.18	Joback Method
cpg	1009.60	J/mol×K	998.72	Joback Method
cpg	1022.82	J/mol×K	1035.27	Joback Method
cpg	1035.11	J/mol×K	1071.82	Joback Method
cpg	1046.57	J/mol×K	1108.37	Joback Method
cpg	1057.28	J/mol×K	1144.91	Joback Method
dvisc	0.0004763	Pa×s	567.35	Joback Method
dvisc	0.0002813	Pa×s	627.06	Joback Method

dvisc	0.0001820	Pa×s	686.78	Joback Method
dvisc	0.0001263	Pa×s	746.49	Joback Method
dvisc	0.0000925	Pa×s	806.20	Joback Method
dvisc	0.0000707	Pa×s	865.92	Joback Method
dvisc	0.0000560	Pa×s	925.63	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=U369884&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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