Diethylmalonic acid, 2-naphthyl nonyl ester

Inchi: InChI=1S/C26H36O4/c1-4-7-8-9-10-11-14-19-29-24(27)26(5-2,6-3)25(28)30-23-18-17-21
InchiKey: JZFRISBRKLQZSZ-UHFFFAOYSA-N
Formula: C26H36O4
SMILES: CCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc2ccccc2c1
Mol. weight [g/mol]: 412.56

Physical Properties

Property code	Value	Unit	Source
gf	-87.53	kJ/mol	Joback Method
hf	-662.19	kJ/mol	Joback Method
hfus	51.93	kJ/mol	Joback Method
hvap	95.06	kJ/mol	Joback Method
log10ws	-8.07		Crippen Method
logp	6.845		Crippen Method
mcvol	348.860	ml/mol	McGowan Method
pc	1080.64	kPa	Joback Method
rinpol	2991.00		NIST Webbook
tb	994.27	K	Joback Method
tc	1219.05	K	Joback Method
tf	601.16	K	Joback Method
vc	1.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1162.32	J/mol×K	994.27	Joback Method
cpg	1178.38	J/mol×K	1031.73	Joback Method
cpg	1193.32	J/mol×K	1069.20	Joback Method
cpg	1207.24	J/mol×K	1106.66	Joback Method
cpg	1220.24	J/mol×K	1144.12	Joback Method
cpg	1232.42	J/mol×K	1181.59	Joback Method
cpg	1243.88	J/mol×K	1219.05	Joback Method
dvisc	0.0003422	Pa×s	601.16	Joback Method
dvisc	0.0001956	Pa×s	666.68	Joback Method

dvisc	0.0001236	Pa×s	732.20	Joback Method
dvisc	0.0000842	Pa×s	797.72	Joback Method
dvisc	0.0000608	Pa×s	863.23	Joback Method
dvisc	0.0000460	Pa×s	928.75	Joback Method
dvisc	0.0000361	Pa×s	994.27	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=U369887&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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