Diethylmalonic acid, 1-naphthyl ethyl ester

Other names: Diethylmalonic acid, 1-naphthyl propyl ester
Inchi: InChI=1S/C19H22O4/c1-4-19(5-2,17(20)22-6-3)18(21)23-16-13-9-11-14-10-7-8-12-15(14
InchiKey: IRWSVMHDBGMBEY-UHFFFAOYSA-N
Formula: C19H22O4
SMILES: CCOC(=O)C(CC)(CC)C(=O)Oc1cccc2ccccc12
Mol. weight [g/mol]: 314.38

Physical Properties

Property code	Value	Unit	Source
gf	-146.47	kJ/mol	Joback Method
hf	-517.71	kJ/mol	Joback Method
hfus	33.80	kJ/mol	Joback Method
hvap	79.48	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	4.115		Crippen Method
mcvol	250.230	ml/mol	McGowan Method
pc	1780.34	kPa	Joback Method
rinpol	2260.00		NIST Webbook
rinpol	2260.00		NIST Webbook
tb	834.11	K	Joback Method
tc	1057.24	K	Joback Method
tf	522.27	K	Joback Method
vc	0.951	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	746.82	J/mol×K	834.11	Joback Method
cpg	809.34	J/mol×K	1020.05	Joback Method
cpg	798.71	J/mol×K	982.86	Joback Method
cpg	787.23	J/mol×K	945.67	Joback Method
cpg	774.80	J/mol×K	908.49	Joback Method
cpg	761.35	J/mol×K	871.30	Joback Method
cpg	819.17	J/mol×K	1057.24	Joback Method

dvisc	0.0000973	Pa×s	834.11	Joback Method
dvisc	0.0001212	Pa×s	782.14	Joback Method
dvisc	0.0001558	Pa×s	730.16	Joback Method
dvisc	0.0002082	Pa×s	678.19	Joback Method
dvisc	0.0002919	Pa×s	626.22	Joback Method
dvisc	0.0004351	Pa×s	574.24	Joback Method
dvisc	0.0007020	Pa×s	522.27	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=U369866&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