Diethylmalonic acid, 1-naphthyl propyl ester

Other names: Diethylmalonic acid, isobutyl 1-naphthyl ester
Inchi: InChI=1S/C20H24O4/c1-4-14-23-18(21)20(5-2,6-3)19(22)24-17-13-9-11-15-10-7-8-12-16
InchiKey: ZTCZPPLLAGOTNX-UHFFFAOYSA-N
Formula: C20H24O4
SMILES: CCCOC(=O)C(CC)(CC)C(=O)Oc1cccc2ccccc12
Mol. weight [g/mol]: 328.40

Physical Properties

Property code	Value	Unit	Source
hfus	36.39	kJ/mol	Joback Method
ie	8.00	eV	Cheméo Relay (1.0)
log10ws	-4.67		Cheméo Relay (1.0)
logp	4.505		Crippen Method
mcvol	264.320	ml/mol	McGowan Method
rinpol	2353.00		NIST Webbook
rinpol	2353.00		NIST Webbook
tb	653.69	K	Cheméo Relay (1.0)
tf	338.55	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	803.94	J/mol×K	856.99	Joback Method
cpg	818.67	J/mol×K	893.84	Joback Method
cpg	832.32	J/mol×K	930.70	Joback Method
cpg	844.95	J/mol×K	967.55	Joback Method
cpg	856.66	J/mol×K	1004.40	Joback Method
cpg	867.50	J/mol×K	1041.25	Joback Method
cpg	877.56	J/mol×K	1078.11	Joback Method
dvisc	0.0006413	Pa×s	533.54	Joback Method
dvisc	0.0003924	Pa×s	587.45	Joback Method
dvisc	0.0002608	Pa×s	641.36	Joback Method
dvisc	0.0001847	Pa×s	695.26	Joback Method
dvisc	0.0001374	Pa×s	749.17	Joback Method

dvisc	0.0001064	Pa×s	803.08	Joback Method
dvisc	0.0000851	Pa×s	856.99	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369867&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point