Diethylmalonic acid, 1-naphthyl undecyl ester

Inchi: InChI=1S/C28H40O4/c1-4-7-8-9-10-11-12-13-16-22-31-26(29)28(5-2,6-3)27(30)32-25-21
InchiKey: AONXADHJLHVCBZ-UHFFFAOYSA-N
Formula: C28H40O4
SMILES: CCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc2ccccc12
Mol. weight [g/mol]: 440.61

Physical Properties

Property code	Value	Unit	Source
gf	-70.69	kJ/mol	Joback Method
hf	-703.47	kJ/mol	Joback Method
hfus	57.11	kJ/mol	Joback Method
hvap	99.52	kJ/mol	Joback Method
log10ws	-8.91		Crippen Method
logp	7.626		Crippen Method
mcvol	377.040	ml/mol	McGowan Method
pc	956.14	kPa	Joback Method
rinpol	3114.00		NIST Webbook
rinpol	3114.00		NIST Webbook
tb	1040.03	K	Joback Method
tc	1273.30	K	Joback Method
tf	623.70	K	Joback Method
vc	1.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1286.66	J/mol×K	1040.03	Joback Method
cpg	1360.10	J/mol×K	1234.43	Joback Method
cpg	1347.26	J/mol×K	1195.55	Joback Method
cpg	1333.62	J/mol×K	1156.67	Joback Method
cpg	1319.05	J/mol×K	1117.79	Joback Method
cpg	1303.44	J/mol×K	1078.91	Joback Method
cpg	1372.27	J/mol×K	1273.30	Joback Method
dvisc	0.0000267	Pa×s	1040.03	Joback Method

dvisc	0.0000342	Pa×s	970.64	Joback Method
dvisc	0.0000455	Pa×s	901.25	Joback Method
dvisc	0.0000635	Pa×s	831.87	Joback Method
dvisc	0.0000943	Pa×s	762.48	Joback Method
dvisc	0.0001515	Pa×s	693.09	Joback Method
dvisc	0.0002703	Pa×s	623.70	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=U369875&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