Diethylmalonic acid, di(2-naphthyl) ester

Inchi: InChI=1S/C27H24O4/c1-3-27(4-2,25(28)30-23-15-13-19-9-5-7-11-21(19)17-23)26(29)31-
InchiKey: ZZSDDHQEFYQWPR-UHFFFAOYSA-N
Formula: C27H24O4
SMILES: CCC(CC)(C(=O)Oc1ccc2ccccc2c1)C(=O)Oc1ccc2ccccc2c1
Mol. weight [g/mol]: 412.48

Physical Properties

Property code	Value	Unit	Source
gf	130.32	kJ/mol	Joback Method
hf	-266.70	kJ/mol	Joback Method
hfus	45.19	kJ/mol	Joback Method
hvap	101.87	kJ/mol	Joback Method
log10ws	-8.37		Crippen Method
logp	6.310		Crippen Method
mcvol	319.730	ml/mol	McGowan Method
pc	1505.81	kPa	Joback Method
rinpol	3540.00		NIST Webbook
tb	1067.79	K	Joback Method
tc	1323.35	K	Joback Method
tf	684.07	K	Joback Method
vc	1.212	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1027.42	J/mol×K	1067.79	Joback Method
cpg	1091.10	J/mol×K	1280.75	Joback Method
cpg	1078.80	J/mol×K	1238.16	Joback Method
cpg	1066.48	J/mol×K	1195.57	Joback Method
cpg	1053.94	J/mol×K	1152.98	Joback Method
cpg	1040.98	J/mol×K	1110.38	Joback Method
cpg	1103.56	J/mol×K	1323.35	Joback Method
dvisc	0.0000719	Pa×s	1067.79	Joback Method
dvisc	0.0000870	Pa×s	1003.84	Joback Method

dvisc	0.0001080	Pa×s	939.88	Joback Method
dvisc	0.0001385	Pa×s	875.93	Joback Method
dvisc	0.0001847	Pa×s	811.98	Joback Method
dvisc	0.0002586	Pa×s	748.02	Joback Method
dvisc	0.0003858	Pa×s	684.07	Joback Method

Sources

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=U369889&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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