Diethylmalonic acid, 2-naphthyl pentyl ester

Inchi: InChI=1S/C22H28O4/c1-4-7-10-15-25-20(23)22(5-2,6-3)21(24)26-19-14-13-17-11-8-9-12
InchiKey: SYJVKEKSZSDAPP-UHFFFAOYSA-N
Formula: C22H28O4
SMILES: CCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc2ccccc2c1
Mol. weight [g/mol]: 356.46

Physical Properties

Property code	Value	Unit	Source
gf	-121.21	kJ/mol	Joback Method
hf	-579.63	kJ/mol	Joback Method
hfus	41.57	kJ/mol	Joback Method
hvap	86.16	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	5.285		Crippen Method
mcvol	292.500	ml/mol	McGowan Method
pc	1415.44	kPa	Joback Method
rinpol	2588.00		NIST Webbook
tb	902.75	K	Joback Method
tc	1121.90	K	Joback Method
tf	556.08	K	Joback Method
vc	1.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	920.61	J/mol×K	902.75	Joback Method
cpg	935.72	J/mol×K	939.27	Joback Method
cpg	949.75	J/mol×K	975.80	Joback Method
cpg	962.77	J/mol×K	1012.32	Joback Method
cpg	974.87	J/mol×K	1048.85	Joback Method
cpg	986.12	J/mol×K	1085.37	Joback Method
cpg	996.61	J/mol×K	1121.90	Joback Method
dvisc	0.0005280	Pa×s	556.08	Joback Method
dvisc	0.0003154	Pa×s	613.86	Joback Method

dvisc	0.0002059	Pa×s	671.64	Joback Method
dvisc	0.0001438	Pa×s	729.41	Joback Method
dvisc	0.0001059	Pa×s	787.19	Joback Method
dvisc	0.0000813	Pa×s	844.97	Joback Method
dvisc	0.0000645	Pa×s	902.75	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=U369883&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