Diethylmalonic acid, isobutyl 2-naphthyl ester

Inchi: InChI=1S/C21H26O4/c1-5-21(6-2,19(22)24-14-15(3)4)20(23)25-18-12-11-16-9-7-8-10-17
InchiKey: IHASQWIZERONMC-UHFFFAOYSA-N
Formula: C21H26O4
SMILES: CCC(CC)(C(=O)OCC(C)C)C(=O)Oc1ccc2ccccc2c1
Mol. weight [g/mol]: 342.43

Physical Properties

Property code	Value	Unit	Source
gf	-132.07	kJ/mol	Joback Method
hf	-564.27	kJ/mol	Joback Method
hfus	35.45	kJ/mol	Joback Method
hvap	83.55	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	4.751		Crippen Method
mcvol	278.410	ml/mol	McGowan Method
pc	1533.06	kPa	Joback Method
rinpol	2454.00		NIST Webbook
rinpol	2454.00		NIST Webbook
tb	879.43	K	Joback Method
tc	1101.76	K	Joback Method
tf	529.81	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	862.41	J/mol×K	879.43	Joback Method
cpg	877.47	J/mol×K	916.49	Joback Method
cpg	891.42	J/mol×K	953.54	Joback Method
cpg	904.32	J/mol×K	990.60	Joback Method
cpg	916.25	J/mol×K	1027.65	Joback Method
cpg	927.31	J/mol×K	1064.71	Joback Method
cpg	937.57	J/mol×K	1101.76	Joback Method
dvisc	0.0006385	Pa×s	529.81	Joback Method

dvisc	0.0003652	Pa×s	588.08	Joback Method
dvisc	0.0002310	Pa×s	646.35	Joback Method
dvisc	0.0001576	Pa×s	704.62	Joback Method
dvisc	0.0001140	Pa×s	762.89	Joback Method
dvisc	0.0000864	Pa×s	821.16	Joback Method
dvisc	0.0000679	Pa×s	879.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369881&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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