Dimethylmalonic acid, isohexyl 2-naphthylmethyl ester

Inchi: InChI=1S/C22H28O4/c1-16(2)8-7-13-25-20(23)22(3,4)21(24)26-15-17-11-12-18-9-5-6-10

InchiKey: QKCMAIFWWUHKAT-UHFFFAOYSA-N

Formula: C22H28O4

SMILES: CC(C)CCCOC(=O)C(C)(C)C(=O)OCc1ccc2ccccc2c1

Mol. weight [g/mol]: 356.46

Physical Properties

Property code	Value	Unit	Source
gf	-123.65	kJ/mol	Joback Method
hf	-584.91	kJ/mol	Joback Method
hfus	38.04	kJ/mol	Joback Method
hvap	85.77	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	4.889		Crippen Method
mcvol	292.500	ml/mol	McGowan Method
pc	1423.99	kPa	Joback Method
rinpol	2606.00		NIST Webbook
rinpol	2606.00		NIST Webbook
tb	902.31	K	Joback Method
tc	1123.67	K	Joback Method
tf	541.08	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	921.11	J/mol×K	902.31	Joback Method
cpg	936.34	J/mol×K	939.20	Joback Method
cpg	950.44	J/mol×K	976.10	Joback Method
cpg	963.51	J/mol×K	1012.99	Joback Method
cpg	975.63	J/mol×K	1049.89	Joback Method
cpg	986.87	J/mol×K	1086.78	Joback Method
cpg	997.33	J/mol×K	1123.67	Joback Method
dvisc	0.0005764	Pa×s	541.08	Joback Method

dvisc	0.0003259	Pa×s	601.29	Joback Method
dvisc	0.0002044	Pa×s	661.49	Joback Method
dvisc	0.0001386	Pa×s	721.69	Joback Method
dvisc	0.0000998	Pa×s	781.90	Joback Method
dvisc	0.0000753	Pa×s	842.11	Joback Method
dvisc	0.0000590	Pa×s	902.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363859&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