Dimethylmalonic acid, 2-naphthylmethyl nonyl ester

Inchi: InChI=1S/C25H34O4/c1-4-5-6-7-8-9-12-17-28-23(26)25(2,3)24(27)29-19-20-15-16-21-13

InchiKey: NABPRQQIUPHGRX-UHFFFAOYSA-N

Formula: C25H34O4

SMILES: CCCCCCCCCOC(=O)C(C)(C)C(=O)OCc1ccc2ccccc2c1

Mol. weight [g/mol]: 398.54

Physical Properties

Property code	Value	Unit	Source
gf	-95.95	kJ/mol	Joback Method
hf	-641.55	kJ/mol	Joback Method
hfus	49.34	kJ/mol	Joback Method
hvap	92.84	kJ/mol	Joback Method
log10ws	-7.50		Crippen Method
logp	6.203		Crippen Method
mcvol	334.770	ml/mol	McGowan Method
pc	1152.22	kPa	Joback Method
rinpol	2934.00		NIST Webbook
rinpol	2934.00		NIST Webbook
tb	971.39	K	Joback Method
tc	1193.44	K	Joback Method
tf	589.89	K	Joback Method
vc	1.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1100.96	J/mol×K	971.39	Joback Method
cpg	1116.74	J/mol×K	1008.40	Joback Method
cpg	1131.41	J/mol×K	1045.41	Joback Method
cpg	1145.07	J/mol×K	1082.41	Joback Method
cpg	1157.80	J/mol×K	1119.42	Joback Method
cpg	1169.72	J/mol×K	1156.43	Joback Method
cpg	1180.90	J/mol×K	1193.44	Joback Method
dvisc	0.0003833	Pa×s	589.89	Joback Method

dvisc	0.0002215	Pa×s	653.47	Joback Method
dvisc	0.0001410	Pa×s	717.06	Joback Method
dvisc	0.0000967	Pa×s	780.64	Joback Method
dvisc	0.0000701	Pa×s	844.22	Joback Method
dvisc	0.0000532	Pa×s	907.81	Joback Method
dvisc	0.0000419	Pa×s	971.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363862&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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