Dimethylmalonic acid, 2-naphthylmethyl undecyl ester

Inchi: InChI=1S/C27H38O4/c1-4-5-6-7-8-9-10-11-14-19-30-25(28)27(2,3)26(29)31-21-22-17-18

InchiKey: DJDLAYOCZLKEHD-UHFFFAOYSA-N

Formula: C27H38O4

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

Mol. weight [g/mol]: 426.59

Physical Properties

Property code	Value	Unit	Source
gf	-79.11	kJ/mol	Joback Method
hf	-682.83	kJ/mol	Joback Method
hfus	54.52	kJ/mol	Joback Method
hvap	97.29	kJ/mol	Joback Method
log10ws	-8.34		Crippen Method
logp	6.983		Crippen Method
mcvol	362.950	ml/mol	McGowan Method
pc	1015.53	kPa	Joback Method
rinpol	3147.00		NIST Webbook
rinpol	3147.00		NIST Webbook
tb	1017.15	K	Joback Method
tc	1245.65	K	Joback Method
tf	612.43	K	Joback Method
vc	1.399	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1224.23	J/mol×K	1017.15	Joback Method
cpg	1240.62	J/mol×K	1055.23	Joback Method
cpg	1255.87	J/mol×K	1093.32	Joback Method
cpg	1270.09	J/mol×K	1131.40	Joback Method
cpg	1283.39	J/mol×K	1169.49	Joback Method
cpg	1295.87	J/mol×K	1207.57	Joback Method
cpg	1307.66	J/mol×K	1245.65	Joback Method
dvisc	0.0003046	Pa×s	612.43	Joback Method

dvisc	0.0001724	Pa×s	679.88	Joback Method
dvisc	0.0001081	Pa×s	747.34	Joback Method
dvisc	0.0000732	Pa×s	814.79	Joback Method
dvisc	0.0000527	Pa×s	882.24	Joback Method
dvisc	0.0000397	Pa×s	949.70	Joback Method
dvisc	0.0000310	Pa×s	1017.15	Joback Method

Sources

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=U363864&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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