Dimethylmalonic acid, nonyl trans-4-methylcyclohexyl ester

Inchi: InChI=1S/C21H38O4/c1-5-6-7-8-9-10-11-16-24-19(22)21(3,4)20(23)25-18-14-12-17(2)13

InchiKey: JIQNHCVCQGPNRL-UHFFFAOYSA-N

Formula: C21H38O4

SMILES: CCCCCCCCCOC(=O)C(C)(C)C(=O)OC1CCC(C)CC1

Mol. weight [g/mol]: 354.52

Physical Properties

Property code	Value	Unit	Source
gf	-322.32	kJ/mol	Joback Method
hf	-941.14	kJ/mol	Joback Method
hfus	41.21	kJ/mol	Joback Method
hvap	79.48	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	5.428		Crippen Method
mcvol	310.770	ml/mol	McGowan Method
pc	1148.32	kPa	Joback Method
rinpol	2304.00		NIST Webbook
rinpol	2304.00		NIST Webbook
tb	844.11	K	Joback Method
tc	1044.78	K	Joback Method
tf	476.31	K	Joback Method
vc	1.181	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.55	J/mol×K	844.11	Joback Method
cpg	1115.64	J/mol×K	1011.33	Joback Method
cpg	1101.47	J/mol×K	977.89	Joback Method
cpg	1086.01	J/mol×K	944.44	Joback Method
cpg	1069.23	J/mol×K	911.00	Joback Method
cpg	1051.09	J/mol×K	877.55	Joback Method
cpg	1128.56	J/mol×K	1044.78	Joback Method
dvisc	0.0000486	Pa×s	844.11	Joback Method

dvisc	0.0000650	Pa×s	782.81	Joback Method
dvisc	0.0000914	Pa×s	721.51	Joback Method
dvisc	0.0001369	Pa×s	660.21	Joback Method
dvisc	0.0002229	Pa×s	598.91	Joback Method
dvisc	0.0004053	Pa×s	537.61	Joback Method
dvisc	0.0008599	Pa×s	476.31	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=U363901&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