Dimethylmalonic acid, decyl nonyl ester

Inchi: InChI=1S/C24H46O4/c1-5-7-9-11-13-15-17-19-21-28-23(26)24(3,4)22(25)27-20-18-16-1
InchiKey: AKYMJUVQIPAIQP-UHFFFAOYSA-N
Formula: C24H46O4
SMILES: CCCCCCCCCCOC(=O)C(C)(C)C(=O)OCCCCCCCCC
Mol. weight [g/mol]: 398.62

Physical Properties

Property code	Value	Unit	Source
gf	-313.80	kJ/mol	Joback Method
hf	-1037.04	kJ/mol	Joback Method
hfus	56.08	kJ/mol	Joback Method
hvap	86.03	kJ/mol	Joback Method
log10ws	-7.35		Crippen Method
logp	6.990		Crippen Method
mcvol	363.900	ml/mol	McGowan Method
pc	859.48	kPa	Joback Method
rinpol	2499.00		NIST Webbook
rinpol	2499.00		NIST Webbook
tb	897.87	K	Joback Method
tc	1099.42	K	Joback Method
tf	506.98	K	Joback Method
vc	1.417	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1217.64	J/mol×K	897.87	Joback Method
cpg	1304.32	J/mol×K	1065.83	Joback Method
cpg	1289.41	J/mol×K	1032.24	Joback Method
cpg	1273.35	J/mol×K	998.65	Joback Method
cpg	1256.06	J/mol×K	965.05	Joback Method
cpg	1237.51	J/mol×K	931.46	Joback Method
cpg	1318.10	J/mol×K	1099.42	Joback Method
dvisc	0.0000228	Pa×s	897.87	Joback Method

dvisc	0.0000311	Pa×s	832.72	Joback Method
dvisc	0.0000447	Pa×s	767.57	Joback Method
dvisc	0.0000686	Pa×s	702.42	Joback Method
dvisc	0.0001149	Pa×s	637.28	Joback Method
dvisc	0.0002166	Pa×s	572.13	Joback Method
dvisc	0.0004804	Pa×s	506.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361708&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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