Dimethylmalonic acid, dodecyl 2-pentyl ester

Inchi: InChI=1S/C22H42O4/c1-6-8-9-10-11-12-13-14-15-16-18-25-20(23)22(4,5)21(24)26-19(3
InchiKey: NMXSWNCLDKZBLB-UHFFFAOYSA-N
Formula: C22H42O4
SMILES: CCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OC(C)CCC
Mol. weight [g/mol]: 370.57

Physical Properties

Property code	Value	Unit	Source
gf	-333.08	kJ/mol	Joback Method
hf	-1001.04	kJ/mol	Joback Method
hfus	47.37	kJ/mol	Joback Method
hvap	81.19	kJ/mol	Joback Method
log10ws	-6.63		Crippen Method
logp	6.209		Crippen Method
mcvol	335.720	ml/mol	McGowan Method
pc	969.88	kPa	Joback Method
rinpol	2286.00		NIST Webbook
tb	851.67	K	Joback Method
tc	1044.13	K	Joback Method
tf	469.44	K	Joback Method
vc	1.298	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1093.02	J/mol×K	851.67	Joback Method
cpg	1112.04	J/mol×K	883.75	Joback Method
cpg	1129.88	J/mol×K	915.82	Joback Method
cpg	1146.58	J/mol×K	947.90	Joback Method
cpg	1162.18	J/mol×K	979.97	Joback Method
cpg	1176.71	J/mol×K	1012.05	Joback Method
cpg	1190.22	J/mol×K	1044.13	Joback Method
dvisc	0.0007385	Pa×s	469.44	Joback Method
dvisc	0.0003111	Pa×s	533.14	Joback Method

dvisc	0.0001576	Pa×s	596.85	Joback Method
dvisc	0.0000910	Pa×s	660.56	Joback Method
dvisc	0.0000579	Pa×s	724.26	Joback Method
dvisc	0.0000396	Pa×s	787.97	Joback Method
dvisc	0.0000287	Pa×s	851.67	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361587&Units=SI

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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