Dimethylmalonic acid, ethyl hexyl ester

Inchi: InChI=1S/C13H24O4/c1-5-7-8-9-10-17-12(15)13(3,4)11(14)16-6-2/h5-10H2,1-4H3
InchiKey: BPWULCWZNSCJSD-UHFFFAOYSA-N
Formula: C13H24O4
SMILES: CCCCCCOC(=O)C(C)(C)C(=O)OCC
Mol. weight [g/mol]: 244.33

Physical Properties

Property code	Value	Unit	Source
gf	-406.42	kJ/mol	Joback Method
hf	-810.00	kJ/mol	Joback Method
hfus	27.59	kJ/mol	Joback Method
hvap	61.55	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.699		Crippen Method
mcvol	208.910	ml/mol	McGowan Method
pc	1803.09	kPa	Joback Method
rinpol	1471.00		NIST Webbook
rinpol	1471.00		NIST Webbook
tb	646.19	K	Joback Method
tc	830.33	K	Joback Method
tf	383.01	K	Joback Method
vc	0.800	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.18	J/mol×K	646.19	Joback Method
cpg	641.60	J/mol×K	799.64	Joback Method
cpg	629.03	J/mol×K	768.95	Joback Method
cpg	615.71	J/mol×K	738.26	Joback Method
cpg	601.65	J/mol×K	707.57	Joback Method
cpg	586.81	J/mol×K	676.88	Joback Method
cpg	653.44	J/mol×K	830.33	Joback Method
dvisc	0.0001172	Pa×s	646.19	Joback Method

dvisc	0.0001555	Pa×s	602.33	Joback Method
dvisc	0.0002158	Pa×s	558.46	Joback Method
dvisc	0.0003166	Pa×s	514.60	Joback Method
dvisc	0.0004990	Pa×s	470.74	Joback Method
dvisc	0.0008633	Pa×s	426.87	Joback Method
dvisc	0.0016936	Pa×s	383.01	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=U361684&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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