Dimethylmalonic acid, heptyl isohexyl ester

Inchi: InChI=1S/C18H34O4/c1-6-7-8-9-10-13-21-16(19)18(4,5)17(20)22-14-11-12-15(2)3/h15H
InchiKey: KQUJGBIKGZBJIV-UHFFFAOYSA-N
Formula: C18H34O4
SMILES: CCCCCCCOC(=O)C(C)(C)C(=O)OCCCC(C)C
Mol. weight [g/mol]: 314.46

Physical Properties

Property code	Value	Unit	Source
gf	-366.76	kJ/mol	Joback Method
hf	-918.48	kJ/mol	Joback Method
hfus	37.01	kJ/mol	Joback Method
hvap	72.29	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.506		Crippen Method
mcvol	279.360	ml/mol	McGowan Method
pc	1251.26	kPa	Joback Method
rinpol	1886.00		NIST Webbook
rinpol	1886.00		NIST Webbook
tb	760.15	K	Joback Method
tc	944.42	K	Joback Method
tf	424.36	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	851.53	J/mol×K	760.15	Joback Method
cpg	869.25	J/mol×K	790.86	Joback Method
cpg	885.98	J/mol×K	821.57	Joback Method
cpg	901.76	J/mol×K	852.29	Joback Method
cpg	916.60	J/mol×K	883.00	Joback Method
cpg	930.53	J/mol×K	913.71	Joback Method
cpg	943.57	J/mol×K	944.42	Joback Method
dvisc	0.0012334	Pa×s	424.36	Joback Method

dvisc	0.0005382	Pa×s	480.32	Joback Method
dvisc	0.0002793	Pa×s	536.29	Joback Method
dvisc	0.0001640	Pa×s	592.25	Joback Method
dvisc	0.0001056	Pa×s	648.22	Joback Method
dvisc	0.0000729	Pa×s	704.18	Joback Method
dvisc	0.0000532	Pa×s	760.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361719&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