Dimethylmalonic acid, heptyl hexyl ester

Inchi: InChI=1S/C18H34O4/c1-5-7-9-11-13-15-22-17(20)18(3,4)16(19)21-14-12-10-8-6-2/h5-15
InchiKey: MGQMQOUJLSQJTI-UHFFFAOYSA-N
Formula: C18H34O4
SMILES: CCCCCCCOC(=O)C(C)(C)C(=O)OCCCCCC
Mol. weight [g/mol]: 314.46

Physical Properties

Property code	Value	Unit	Source
gf	-364.32	kJ/mol	Joback Method
hf	-913.20	kJ/mol	Joback Method
hfus	40.54	kJ/mol	Joback Method
hvap	72.68	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.650		Crippen Method
mcvol	279.360	ml/mol	McGowan Method
pc	1244.21	kPa	Joback Method
rinpol	1925.00		NIST Webbook
rinpol	1925.00		NIST Webbook
tb	760.59	K	Joback Method
tc	943.17	K	Joback Method
tf	439.36	K	Joback Method
vc	1.081	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	851.04	J/mol×K	760.59	Joback Method
cpg	868.59	J/mol×K	791.02	Joback Method
cpg	885.17	J/mol×K	821.45	Joback Method
cpg	900.82	J/mol×K	851.88	Joback Method
cpg	915.57	J/mol×K	882.31	Joback Method
cpg	929.42	J/mol×K	912.74	Joback Method
cpg	942.42	J/mol×K	943.17	Joback Method
dvisc	0.0010148	Pa×s	439.36	Joback Method

dvisc	0.0004855	Pa×s	492.90	Joback Method
dvisc	0.0002684	Pa×s	546.44	Joback Method
dvisc	0.0001649	Pa×s	599.97	Joback Method
dvisc	0.0001097	Pa×s	653.51	Joback Method
dvisc	0.0000777	Pa×s	707.05	Joback Method
dvisc	0.0000577	Pa×s	760.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361689&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