

Dimethylmalonic acid, heptyl 2-methylpent-3-yl ester

Inchi:	InChI=1S/C18H34O4/c1-7-9-10-11-12-13-21-16(19)18(5,6)17(20)22-15(8-2)14(3)4/h14-1
InchiKey:	ZEMIEVXOXHYVJU-UHFFFAOYSA-N
Formula:	C18H34O4
SMILES:	CCCCCCCOC(=O)C(C)(C)C(=O)OC(CC)C(C)C
Mol. weight [g/mol]:	314.46

Physical Properties

Property code	Value	Unit	Source
gf	-369.20	kJ/mol	Joback Method
hf	-923.76	kJ/mol	Joback Method
hfus	33.49	kJ/mol	Joback Method
hvap	71.90	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	4.504		Crippen Method
mcvol	279.360	ml/mol	McGowan Method
pc	1258.37	kPa	Joback Method
rinsol	1876.00		NIST Webbook
tb	759.71	K	Joback Method
tc	945.81	K	Joback Method
tf	409.36	K	Joback Method
vc	1.069	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	852.02	J/molxK	759.71	Joback Method
cpg	869.92	J/molxK	790.73	Joback Method
cpg	886.82	J/molxK	821.74	Joback Method
cpg	902.72	J/molxK	852.76	Joback Method
cpg	917.67	J/molxK	883.78	Joback Method
cpg	931.67	J/molxK	914.80	Joback Method
cpg	944.77	J/molxK	945.81	Joback Method
dvisc	0.0015357	Paxs	409.36	Joback Method
dvisc	0.0006044	Paxs	467.75	Joback Method

dvisc	0.0002925	Paxs	526.14	Joback Method
dvisc	0.0001637	Paxs	584.54	Joback Method
dvisc	0.0001018	Paxs	642.93	Joback Method
dvisc	0.0000685	Paxs	701.32	Joback Method
dvisc	0.0000490	Paxs	759.71	Joback Method

Sources

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=U361792&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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