

Dimethylmalonic acid, isobutyl 4-octyl ester

Inchi:	InChI=1S/C17H32O4/c1-7-9-11-14(10-8-2)21-16(19)17(5,6)15(18)20-12-13(3)4/h13-14H
InchiKey:	AIJBGEYNDVJYOQ-UHFFFAOYSA-N
Formula:	C17H32O4
SMILES:	CCCCC(CCC)OC(=O)C(C)(C)C(=O)OCC(C)C
Mol. weight [g/mol]:	300.43

Physical Properties

Property code	Value	Unit	Source
gf	-377.62	kJ/mol	Joback Method
hf	-903.12	kJ/mol	Joback Method
hfus	30.90	kJ/mol	Joback Method
hvap	69.68	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	4.114		Crippen Method
mcvol	265.270	ml/mol	McGowan Method
pc	1348.67	kPa	Joback Method
rinsol	1674.00		NIST Webbook
tb	736.83	K	Joback Method
tc	922.80	K	Joback Method
tf	398.09	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.82	J/molxK	736.83	Joback Method
cpg	811.45	J/molxK	767.82	Joback Method
cpg	828.10	J/molxK	798.82	Joback Method
cpg	843.79	J/molxK	829.81	Joback Method
cpg	858.54	J/molxK	860.81	Joback Method
cpg	872.39	J/molxK	891.80	Joback Method
cpg	885.36	J/molxK	922.80	Joback Method
dvisc	0.0017460	Paxs	398.09	Joback Method
dvisc	0.0006925	Paxs	454.55	Joback Method

dvisc	0.0003369	Paxs	511.00	Joback Method
dvisc	0.0001892	Paxs	567.46	Joback Method
dvisc	0.0001179	Paxs	623.92	Joback Method
dvisc	0.0000795	Paxs	680.37	Joback Method
dvisc	0.0000570	Paxs	736.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361731&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
mccvol:	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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