

Dimethyl 2-hydroxy-2-methylbutane-1,4-dioate

Inchi:	InChI=1S/C7H12O5/c1-7(10,6(9)12-3)4-5(8)11-2/h10H,4H2,1-3H3
InchiKey:	GMSSNUSBKDUVFC-UHFFFAOYSA-N
Formula:	C7H12O5
SMILES:	COC(=O)CC(C)(O)C(=O)OC
Mol. weight [g/mol]:	176.17
CAS:	19020-62-3

Physical Properties

Property code	Value	Unit	Source
gf	-593.76	kJ/mol	Joback Method
hf	-838.39	kJ/mol	Joback Method
hfus	16.13	kJ/mol	Joback Method
hvap	64.87	kJ/mol	Joback Method
log10ws	0.15		Crippen Method
logp	-0.527		Crippen Method
mcvol	130.240	ml/mol	McGowan Method
pc	3513.74	kPa	Joback Method
rinpol	1115.50		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	1087.00		NIST Webbook
tb	601.09	K	Joback Method
tc	787.29	K	Joback Method
tf	376.21	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.87	J/molxK	601.09	Joback Method
cpg	371.63	J/molxK	756.26	Joback Method
cpg	364.03	J/molxK	725.22	Joback Method
cpg	355.95	J/molxK	694.19	Joback Method
cpg	347.41	J/molxK	663.16	Joback Method
cpg	338.38	J/molxK	632.12	Joback Method

cpg	378.78	J/mol×K	787.29	Joback Method
dvisc	0.0000742	Paxs	601.09	Joback Method
dvisc	0.0001113	Paxs	563.61	Joback Method
dvisc	0.0001768	Paxs	526.13	Joback Method
dvisc	0.0003018	Paxs	488.65	Joback Method
dvisc	0.0005629	Paxs	451.17	Joback Method
dvisc	0.0011753	Paxs	413.69	Joback Method
dvisc	0.0028417	Paxs	376.21	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19020623&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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