

3,3-Dimethoxy-2-butanone

Inchi:	InChI=1S/C6H12O3/c1-5(7)6(2,8-3)9-4/h1-4H3
InchiKey:	UFQBSPGKRRSATO-UHFFFAOYSA-N
Formula:	C6H12O3
SMILES:	COC(C)(OC)C(C)=O
Mol. weight [g/mol]:	132.16
CAS:	21983-72-2

Physical Properties

Property code	Value	Unit	Source
gf	-336.44	kJ/mol	Joback Method
hf	-552.94	kJ/mol	Joback Method
hfus	7.86	kJ/mol	Joback Method
hvap	39.22	kJ/mol	Joback Method
log10ws	-0.40		Crippen Method
logp	0.584		Crippen Method
mcvol	108.710	ml/mol	McGowan Method
pc	3280.28	kPa	Joback Method
tb	418.70	K	NIST Webbook
tc	621.06	K	Joback Method
tf	254.19	K	Joback Method
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.41	J/molxK	432.16	Joback Method
cpg	235.24	J/molxK	463.64	Joback Method
cpg	245.64	J/molxK	495.13	Joback Method
cpg	255.63	J/molxK	526.61	Joback Method
cpg	265.19	J/molxK	558.09	Joback Method
cpg	274.33	J/molxK	589.58	Joback Method
cpg	283.05	J/molxK	621.06	Joback Method
dvisc	0.0033807	Paxs	254.19	Joback Method
dvisc	0.0017467	Paxs	283.85	Joback Method

dvisc	0.0010226	Paxs	313.51	Joback Method
dvisc	0.0006567	Paxs	343.17	Joback Method
dvisc	0.0004525	Paxs	372.84	Joback Method
dvisc	0.0003294	Paxs	402.50	Joback Method
dvisc	0.0002505	Paxs	432.16	Joback Method

Sources

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=C21983722&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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