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

Physical Properties

Property code	Value	Unit	Source
hf	-551.61	kJ/mol	Cheméo Relay (1.0)
hfus	7.86	kJ/mol	Joback Method
hvap	44.08	kJ/mol	Cheméo Relay (1.0)
ie	9.13	eV	Cheméo Relay (1.0)
log10ws	-0.40		Cheméo Relay (1.0)
logp	0.584		Crippen Method
mcvol	108.710	ml/mol	McGowan Method
tb	418.70	K	NIST Webbook
tc	594.15	K	Cheméo Relay (1.0)
tf	281.37	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.41	J/mol×K	432.16	Joback Method
cpg	283.05	J/mol×K	621.06	Joback Method
cpg	274.33	J/mol×K	589.58	Joback Method
cpg	265.19	J/mol×K	558.09	Joback Method
cpg	255.63	J/mol×K	526.61	Joback Method
cpg	245.64	J/mol×K	495.13	Joback Method
cpg	235.24	J/mol×K	463.64	Joback Method
dvisc	0.0006567	Pa×s	343.17	Joback Method
dvisc	0.0002505	Pa×s	432.16	Joback Method
dvisc	0.0003294	Pa×s	402.50	Joback Method
dvisc	0.0004525	Pa×s	372.84	Joback Method
dvisc	0.0033807	Pa×s	254.19	Joback Method

dvisc	0.0010226	Pa×s	313.51	Joback Method
dvisc	0.0017467	Pa×s	283.85	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C21983722&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point