3,3-Dimethyl-tetrahydrofuran

Inchi: InChI=1S/C6H12O/c1-6(2)3-4-7-5-6/h3-5H2,1-2H3
InchiKey: WDKUXUZYKCXAHC-UHFFFAOYSA-N
Formula: C6H12O
SMILES: CC1(C)CCOC1
Mol. weight [g/mol]: 100.16

Physical Properties

Property code	Value	Unit	Source
gf	-55.42	kJ/mol	Joback Method
hf	-223.45	kJ/mol	Joback Method
hfus	6.91	kJ/mol	Joback Method
hvap	32.57	kJ/mol	Joback Method
log10ws	-1.07		Crippen Method
logp	1.433		Crippen Method
mcvol	90.410	ml/mol	McGowan Method
pc	4015.93	kPa	Joback Method
rinpol	737.00		NIST Webbook
tb	379.15	K	Joback Method
tc	584.69	K	Joback Method
tf	218.75	K	Joback Method
vc	0.332	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.14	J/mol×K	379.15	Joback Method
cpg	180.73	J/mol×K	413.41	Joback Method
cpg	194.23	J/mol×K	447.66	Joback Method
cpg	206.73	J/mol×K	481.92	Joback Method
cpg	218.32	J/mol×K	516.18	Joback Method
cpg	229.09	J/mol×K	550.44	Joback Method
cpg	239.15	J/mol×K	584.69	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=R405842&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
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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