

2-Butyl-2-methyl tetrahydrofuran

Inchi:	InChI=1S/C10H20O/c1-4-5-7-10(3)8-6-9(2)11-10/h9H,4-8H2,1-3H3
InchiKey:	CQAKVJVSUDPXDY-UHFFFAOYSA-N
Formula:	C10H20O
SMILES:	CCCCC1(C)CCC(C)O1
Mol. weight [g/mol]:	156.27

Physical Properties

Property code	Value	Unit	Source
gf	-29.45	kJ/mol	Joback Method
hf	-326.35	kJ/mol	Joback Method
hfus	18.34	kJ/mol	Joback Method
hvap	41.16	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	3.134		Crippen Method
mcvol	146.770	ml/mol	McGowan Method
pc	2512.55	kPa	Joback Method
rinpol	1005.00		NIST Webbook
tb	466.00	K	Joback Method
tc	662.84	K	Joback Method
tf	259.59	K	Joback Method
vc	0.554	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.82	J/mol×K	466.00	Joback Method
cpg	353.24	J/mol×K	498.81	Joback Method
cpg	370.58	J/mol×K	531.61	Joback Method
cpg	386.93	J/mol×K	564.42	Joback Method
cpg	402.38	J/mol×K	597.23	Joback Method
cpg	417.02	J/mol×K	630.03	Joback Method
cpg	430.92	J/mol×K	662.84	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=R405713&Units=SI

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
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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