

3-Butyn-2-ol, 2-(1-methylcyclopropyl)-

Inchi:	InChI=1S/C8H12O/c1-4-8(3,9)7(2)5-6-7/h1,9H,5-6H2,2-3H3
InchiKey:	MWOFUOAWMMDAHZ-UHFFFAOYSA-N
Formula:	C8H12O
SMILES:	C#CC(C)(O)C1(C)CC1
Mol. weight [g/mol]:	124.18
CAS:	98558-09-9

Physical Properties

Property code	Value	Unit	Source
gf	160.83	kJ/mol	Joback Method
hf	10.51	kJ/mol	Joback Method
hfus	7.96	kJ/mol	Joback Method
hvap	47.41	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	1.171		Crippen Method
mcvol	109.990	ml/mol	McGowan Method
pc	4151.61	kPa	Joback Method
tb	468.49	K	Joback Method
tc	671.13	K	Joback Method
tf	331.97	K	Joback Method
vc	0.408	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.93	J/molxK	468.49	Joback Method
cpg	259.12	J/molxK	502.26	Joback Method
cpg	270.21	J/molxK	536.04	Joback Method
cpg	280.32	J/molxK	569.81	Joback Method
cpg	289.59	J/molxK	603.59	Joback Method
cpg	298.16	J/molxK	637.36	Joback Method
cpg	306.15	J/molxK	671.13	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=C98558099&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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