

1-Butene, 3-methyl-2-(1-methylpropoxy)-

Other names:	2-Sec-butoxy-3-methyl-1-butene
Inchi:	InChI=1S/C9H18O/c1-6-8(4)10-9(5)7(2)3/h7-8H,5-6H2,1-4H3
InchiKey:	XAJRFKUYOLUIIB-UHFFFAOYSA-N
Formula:	C9H18O
SMILES:	C=C(OC(C)CC)C(C)C
Mol. weight [g/mol]:	142.24
CAS:	56798-16-4

Physical Properties

Property code	Value	Unit	Source
gf	-5.69	kJ/mol	Joback Method
hf	-256.23	kJ/mol	Joback Method
hfus	10.62	kJ/mol	Joback Method
hvap	36.67	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.971		Crippen Method
mcvol	139.240	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
tb	423.42	K	Joback Method
tc	600.72	K	Joback Method
tf	167.70	K	Joback Method
vc	0.527	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.78	J/molxK	423.42	Joback Method
cpg	297.05	J/molxK	452.97	Joback Method
cpg	310.79	J/molxK	482.52	Joback Method
cpg	324.00	J/molxK	512.07	Joback Method
cpg	336.69	J/molxK	541.62	Joback Method
cpg	348.88	J/molxK	571.17	Joback Method
cpg	360.57	J/molxK	600.72	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C56798164&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
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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