

2-Methoxy-1-butene

Inchi:	InChI=1S/C5H10O/c1-4-5(2)6-3/h2,4H2,1,3H3
InchiKey:	TXTDTCYVDJMLRP-UHFFFAOYSA-N
Formula:	C5H10O
SMILES:	C=C(CC)OC
Mol. weight [g/mol]:	86.13
CAS:	25022-43-9

Physical Properties

Property code	Value	Unit	Source
gf	-34.49	kJ/mol	Joback Method
hf	-163.11	kJ/mol	Joback Method
hfus	7.30	kJ/mol	Joback Method
hvap	28.54	kJ/mol	Joback Method
log10ws	-1.35		Crippen Method
logp	1.556		Crippen Method
mvol	82.880	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
tb	332.78	K	Joback Method
tc	503.98	K	Joback Method
tf	152.62	K	Joback Method
vc	0.316	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	135.27	J/mol×K	332.78	Joback Method
cpg	143.47	J/mol×K	361.31	Joback Method
cpg	151.43	J/mol×K	389.85	Joback Method
cpg	159.15	J/mol×K	418.38	Joback Method
cpg	166.63	J/mol×K	446.91	Joback Method
cpg	173.87	J/mol×K	475.44	Joback Method
cpg	180.88	J/mol×K	503.98	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=C25022439&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
mccvol:	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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