

3-Butenyl, 2-methylene-

Inchi:	InChI=1S/C5H7/c1-4-5(2)3/h4H,1-3H2
InchiKey:	YWCXSTMXMNOMGL-UHFFFAOYSA-N
Formula:	C5H7
SMILES:	[CH2]C(=C)C=C
Mol. weight [g/mol]:	67.11
CAS:	31922-49-3

Physical Properties

Property code	Value	Unit	Source
gf	210.73	kJ/mol	Joback Method
hf	150.35	kJ/mol	Joback Method
hfus	6.52	kJ/mol	Joback Method
hvap	25.32	kJ/mol	Joback Method
ie	7.90	eV	NIST Webbook
log10ws	-1.23		Crippen Method
logp	1.563		Crippen Method
mcvol	70.560	ml/mol	McGowan Method
pc	4082.92	kPa	Joback Method
tb	306.34	K	Joback Method
tc	476.11	K	Joback Method
tf	145.00	K	Joback Method
vc	0.270	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	96.53	J/mol×K	306.34	Joback Method
cpg	104.41	J/mol×K	334.64	Joback Method
cpg	111.80	J/mol×K	362.93	Joback Method
cpg	118.72	J/mol×K	391.23	Joback Method
cpg	125.19	J/mol×K	419.52	Joback Method
cpg	131.25	J/mol×K	447.82	Joback Method
cpg	136.92	J/mol×K	476.11	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C31922493&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
ie:	Ionization energy
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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