2-Butenal,2-methyl-(Z)-

Inchi: InChI=1S/C5H8O/c1-3-5(2)4-6/h3-4H,1-2H3/b5-3-
InchiKey: ACWQBUSCFPJUPN-HYXAFXHYSA-N
Formula: C5H8O
SMILES: CC=C(C)C=O
Mol. weight [g/mol]: 84.12
CAS: 6038-09-1

Physical Properties

Property code	Value	Unit	Source
affp	843.90	kJ/mol	NIST Webbook
basg	812.10	kJ/mol	NIST Webbook
gf	-36.63	kJ/mol	Joback Method
hf	-124.68	kJ/mol	Joback Method
hfus	9.89	kJ/mol	Joback Method
hvap	33.48	kJ/mol	Joback Method
ie	9.59	eV	NIST Webbook
log10ws	-1.05		Crippen Method
logp	1.151		Crippen Method
mcvol	78.580	ml/mol	McGowan Method
pc	4072.51	kPa	Joback Method
tb	366.50	K	Joback Method
tc	552.54	K	Joback Method
tf	169.07	K	Joback Method
vc	0.314	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	130.05	J/mol×K	366.50	Joback Method
cpg	138.26	J/mol×K	397.51	Joback Method
cpg	146.07	J/mol×K	428.51	Joback Method
cpg	153.48	J/mol×K	459.52	Joback Method
cpg	160.51	J/mol×K	490.53	Joback Method
cpg	167.19	J/mol×K	521.53	Joback Method

cpg	173.52	J/mol×K	552.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6038091&Units=SI
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

Legend

affp:	Proton affinity
basg:	Gas basicity
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