1,2-Butadienone, 3-methyl-

Inchi: InChI=1S/C5H6O/c1-5(2)3-4-6/h1-2H3
InchiKey: CULFHGAEORKRLD-UHFFFAOYSA-N
Formula: C5H6O
SMILES: CC(C)=C=C=O
Mol. weight [g/mol]: 82.10
CAS: 63364-70-5

Physical Properties

Property code	Value	Unit	Source
gf	80.89	kJ/mol	Joback Method
hf	36.05	kJ/mol	Joback Method
hfus	17.06	kJ/mol	Joback Method
hvap	33.41	kJ/mol	Joback Method
ie	8.65	eV	NIST Webbook
log10ws	-5.58		Crippen Method
logp	0.939		Crippen Method
mcvol	74.280	ml/mol	McGowan Method
pc	5327.93	kPa	Joback Method
tb	311.10	K	Joback Method
tc	487.78	K	Joback Method
tf	161.08	K	Joback Method
vc	0.293	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	115.20	J/mol×K	311.10	Joback Method
cpg	121.32	J/mol×K	340.55	Joback Method
cpg	127.21	J/mol×K	369.99	Joback Method
cpg	132.88	J/mol×K	399.44	Joback Method
cpg	138.32	J/mol×K	428.88	Joback Method
cpg	143.55	J/mol×K	458.33	Joback Method
cpg	148.56	J/mol×K	487.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C63364705&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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