Bicyclo(3.3.1)nonane-2,6-dione

Other names:	Bicyclo[3.3.1]nona-2,6-dione
	Meerwein's ketone
Inchi:	InChI=1S/C9H12O2/c10-8-3-1-6-5-7(8)2-4-9(6)11/h6-7H,1-5H2
InchiKey:	QWNPVTXLBMSEPN-UHFFFAOYSA-N
Formula:	C9H12O2
SMILES:	O=C1CCC2CC1CCC2=O
Mol. weight [g/mol]:	152.19
CAS:	16473-11-3

Physical Properties

Property code	Value	Unit	Source
gf	-135.08	kJ/mol	Joback Method
hf	-377.37	kJ/mol	Joback Method
hfus	8.06	kJ/mol	Joback Method
hvap	44.46	kJ/mol	Joback Method
ie	9.00	eV	NIST Webbook
ie	9.33	eV	NIST Webbook
ie	9.33	eV	NIST Webbook
log10ws	-1.46		Crippen Method
logp	1.335		Crippen Method
mcvol	119.090	ml/mol	McGowan Method
pc	3555.77	kPa	Joback Method
tb	567.25	K	Joback Method
tc	818.08	K	Joback Method
tf	352.95	K	Joback Method
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.15	J/mol×K	567.25	Joback Method
cpg	327.76	J/mol×K	609.05	Joback Method
cpg	345.25	J/mol×K	650.86	Joback Method
cpg	361.62	J/mol×K	692.66	Joback Method

cpg	376.86	J/mol×K	734.47	Joback Method
cpg	390.97	J/mol×K	776.27	Joback Method
cpg	403.93	J/mol×K	818.08	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=C16473113&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