Pentanenitrile, 4,4-dimethyl-5-oxo-

Other names: Butyraldehyde, 4-cyano-2,2-dimethyl
4-formyl-4-methylvaleronitrile
Inchi: InChI=1S/C7H11NO/c1-7(2,6-9)4-3-5-8/h6H,3-4H2,1-2H3
InchiKey: HKJVKIURQSVEQB-UHFFFAOYSA-N
Formula: C7H11NO
SMILES: CC(C)(C=O)CCC#N
Mol. weight [g/mol]: 125.17
CAS: 6140-61-0

Physical Properties

Property code	Value	Unit	Source
gf	44.56	kJ/mol	Joback Method
hf	-117.26	kJ/mol	Joback Method
hfus	10.27	kJ/mol	Joback Method
hvap	47.08	kJ/mol	Joback Method
log10ws	-1.66		Crippen Method
logp	1.515		Crippen Method
mcvol	112.440	ml/mol	McGowan Method
pc	3012.33	kPa	Joback Method
tb	507.07	K	Joback Method
tc	711.25	K	Joback Method
tf	278.06	K	Joback Method
vc	0.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.88	J/mol×K	507.07	Joback Method
cpg	259.14	J/mol×K	541.10	Joback Method
cpg	268.76	J/mol×K	575.13	Joback Method
cpg	277.79	J/mol×K	609.16	Joback Method
cpg	286.26	J/mol×K	643.19	Joback Method
cpg	294.20	J/mol×K	677.22	Joback Method
cpg	301.63	J/mol×K	711.25	Joback Method

Sources

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=C6140610&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume