

5-OXOHEXANENITRILE

Other names:	Hexanenitrile, 5-oxo-5-oxohexanonitrile
Inchi:	InChI=1S/C6H9NO/c1-6(8)4-2-3-5-7/h2-4H2,1H3
InchiKey:	AEVMBQIIZGKQRB-UHFFFAOYSA-N
Formula:	C6H9NO
SMILES:	CC(=O)CCCC#N
Mol. weight [g/mol]:	111.14

Physical Properties

Property code	Value	Unit	Source
af	0.5093		Cheméo Relay (1.0)
hf	-116.56	kJ/mol	Cheméo Relay (1.0)
hfus	14.40	kJ/mol	Joback Method
hvap	58.60	kJ/mol	Cheméo Relay (1.0)
ie	10.36	eV	Cheméo Relay (1.0)
log10ws	0.11		Cheméo Relay (1.0)
logp	1.269		Crippen Method
mcvol	98.350	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
tb	492.03	K	Cheméo Relay (1.0)
tc	669.95	K	Cheméo Relay (1.0)
tf	291.23	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	202.55	J/mol×K	492.63	Joback Method
cpg	211.13	J/mol×K	525.88	Joback Method
cpg	219.30	J/mol×K	559.13	Joback Method
cpg	227.08	J/mol×K	592.38	Joback Method
cpg	234.48	J/mol×K	625.63	Joback Method
cpg	241.50	J/mol×K	658.88	Joback Method
cpg	248.17	J/mol×K	692.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10412983&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
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

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