

Heptanenitrile, 7-hydroxy-

Other names:	7-hydroxyheptane-1-nitrile
Inchi:	InChI=1S/C7H13NO/c8-6-4-2-1-3-5-7-9/h9H,1-5,7H2
InchiKey:	XAZAHJGDOHGFBV-UHFFFAOYSA-N
Formula:	C7H13NO
SMILES:	N#CCCCCCCO
Mol. weight [g/mol]:	127.18
CAS:	17976-80-6

Physical Properties

Property code	Value	Unit	Source
gf	4.42	kJ/mol	Joback Method
hf	-175.16	kJ/mol	Joback Method
hfus	19.48	kJ/mol	Joback Method
hvap	58.33	kJ/mol	Joback Method
log10ws	-1.88		Crippen Method
logp	1.453		Crippen Method
mcvol	116.740	ml/mol	McGowan Method
pc	3009.03	kPa	Joback Method
tb	553.82	K	Joback Method
tc	732.00	K	Joback Method
tf	294.46	K	Joback Method
vc	0.472	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.46	J/mol×K	553.82	Joback Method
cpg	284.54	J/mol×K	583.52	Joback Method
cpg	293.22	J/mol×K	613.21	Joback Method
cpg	301.51	J/mol×K	642.91	Joback Method
cpg	309.44	J/mol×K	672.61	Joback Method
cpg	317.00	J/mol×K	702.30	Joback Method
cpg	324.22	J/mol×K	732.00	Joback Method

Sources

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=C17976806&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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