3-hydroxy-4-pentenenitrile

Inchi: InChI=1S/C5H7NO/c1-2-3-5(7)4-6/h2,5,7H,1,3H2
InchiKey: YFJKKUYODGCDDF-UHFFFAOYSA-N
Formula: C5H7NO
SMILES: C=CCC(O)C#N
Mol. weight [g/mol]: 97.12

Physical Properties

Property code	Value	Unit	Source
gf	72.98	kJ/mol	Joback Method
hf	-13.73	kJ/mol	Joback Method
hfus	9.50	kJ/mol	Joback Method
hvap	52.82	kJ/mol	Joback Method
log10ws	-1.01		Crippen Method
logp	0.447		Crippen Method
mcvol	84.260	ml/mol	McGowan Method
pc	4000.70	kPa	Joback Method
ripol	1345.00		NIST Webbook
ripol	1345.00		NIST Webbook
tb	504.30	K	Joback Method
tc	693.46	K	Joback Method
tf	255.16	K	Joback Method
vc	0.336	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.78	J/mol×K	504.30	Joback Method
cpg	180.23	J/mol×K	535.83	Joback Method
cpg	186.35	J/mol×K	567.35	Joback Method
cpg	192.17	J/mol×K	598.88	Joback Method
cpg	197.68	J/mol×K	630.40	Joback Method
cpg	202.91	J/mol×K	661.93	Joback Method
cpg	207.87	J/mol×K	693.46	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=R512584&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume