5-Cyano-1-pentene

Inchi: InChI=1S/C6H9N/c1-2-3-4-5-6-7/h2H,1,3-5H2
InchiKey: UNAQSRLBVVDYGP-UHFFFAOYSA-N
Formula: C6H9N
SMILES: C=CCCCC#N
Mol. weight [g/mol]: 95.14
CAS: 5048-19-1

Physical Properties

Property code	Value	Unit	Source
gf	220.66	kJ/mol	Joback Method
hf	123.14	kJ/mol	Joback Method
hfus	11.52	kJ/mol	Joback Method
hvap	38.76	kJ/mol	Joback Method
log10ws	-2.05		Crippen Method
logp	1.866		Crippen Method
mcvol	92.480	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
rinpol	857.90		NIST Webbook
rinpol	857.90		NIST Webbook
tb	435.44	K	Joback Method
tc	628.43	K	Joback Method
tf	220.61	K	Joback Method
vc	0.379	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	174.25	J/mol×K	435.44	Joback Method
cpg	182.81	J/mol×K	467.60	Joback Method
cpg	190.97	J/mol×K	499.77	Joback Method
cpg	198.75	J/mol×K	531.93	Joback Method
cpg	206.15	J/mol×K	564.10	Joback Method
cpg	213.19	J/mol×K	596.26	Joback Method
cpg	219.88	J/mol×K	628.43	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=C5048191&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume