5-Hexenenitrile, 2-methyl-

Other names: 2-Methyl 5-hexenenitrile
Inchi: InChI=1S/C7H11N/c1-3-4-5-7(2)6-8/h3,7H,1,4-5H2,2H3
InchiKey: WSLQODBTEPJISE-UHFFFAOYSA-N
Formula: C7H11N
SMILES: C=CCCC(C)C#N
Mol. weight [g/mol]: 109.17
CAS: 30316-00-8

Physical Properties

Property code	Value	Unit	Source
gf	226.64	kJ/mol	Joback Method
hf	97.22	kJ/mol	Joback Method
hfus	10.59	kJ/mol	Joback Method
hvap	40.60	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	2.112		Crippen Method
mcvol	106.570	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
rinpol	848.00		NIST Webbook
rinpol	848.00		NIST Webbook
tb	457.88	K	Joback Method
tc	653.24	K	Joback Method
tf	216.88	K	Joback Method
vc	0.428	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.90	J/mol×K	457.88	Joback Method
cpg	223.04	J/mol×K	490.44	Joback Method
cpg	232.69	J/mol×K	523.00	Joback Method
cpg	241.87	J/mol×K	555.56	Joback Method
cpg	250.60	J/mol×K	588.12	Joback Method
cpg	258.89	J/mol×K	620.68	Joback Method

cpg	266.75	J/mol×K	653.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30316008&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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