Hexanenitrile, 2-methyl

Inchi: InChI=1S/C7H13N/c1-3-4-5-7(2)6-8/h7H,3-5H2,1-2H3
InchiKey: PZYFAYMXLISRGL-UHFFFAOYSA-N
Formula: C7H13N
SMILES: CCCCC(C)C#N
Mol. weight [g/mol]: 111.18

Physical Properties

Property code	Value	Unit	Source
gf	138.80	kJ/mol	Joback Method
hf	-28.21	kJ/mol	Joback Method
hfus	11.87	kJ/mol	Joback Method
hvap	41.27	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.336		Crippen Method
mcvol	110.870	ml/mol	McGowan Method
pc	2749.78	kPa	Joback Method
rinpol	913.00		NIST Webbook
tb	461.20	K	Joback Method
tc	652.47	K	Joback Method
tf	218.64	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.35	J/mol×K	461.20	Joback Method
cpg	240.19	J/mol×K	493.08	Joback Method
cpg	250.55	J/mol×K	524.96	Joback Method
cpg	260.46	J/mol×K	556.84	Joback Method
cpg	269.92	J/mol×K	588.72	Joback Method
cpg	278.94	J/mol×K	620.60	Joback Method
cpg	287.54	J/mol×K	652.47	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R511734&Units=SI

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