

6-(Methylthio)hexanenitrile

Inchi:	InChI=1S/C7H13NS/c1-9-7-5-3-2-4-6-8/h2-5,7H2,1H3
InchiKey:	ULSCBSNSXYDREI-UHFFFAOYSA-N
Formula:	C7H13NS
SMILES:	CSCCCCCC#N
Mol. weight [g/mol]:	143.25
CAS:	72931-29-4

Physical Properties

Property code	Value	Unit	Source
gf	174.36	kJ/mol	Joback Method
hf	18.94	kJ/mol	Joback Method
hfus	19.52	kJ/mol	Joback Method
hvap	48.47	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	2.433		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	2775.92	kPa	Joback Method
rinpol	1306.00		NIST Webbook
rinpol	1317.80		NIST Webbook
rinpol	1306.00		NIST Webbook
rinpol	1317.80		NIST Webbook
ripol	2089.00		NIST Webbook
ripol	2089.00		NIST Webbook
tb	530.42	K	Joback Method
tc	737.50	K	Joback Method
tf	268.04	K	Joback Method
vc	0.507	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.61	J/molxK	530.42	Joback Method
cpg	286.64	J/molxK	564.93	Joback Method
cpg	297.13	J/molxK	599.45	Joback Method

cpg	307.11	J/mol×K	633.96	Joback Method
cpg	316.58	J/mol×K	668.47	Joback Method
cpg	325.55	J/mol×K	702.99	Joback Method
cpg	334.03	J/mol×K	737.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72931294&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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