

7-Methylthioheptanenitrile

Inchi:	InChI=1S/C8H15NS/c1-10-8-6-4-2-3-5-7-9/h2-6,8H2,1H3
InchiKey:	MAMGGQVRQMBXMB-UHFFFAOYSA-N
Formula:	C8H15NS
SMILES:	CSCCCCCC#N
Mol. weight [g/mol]:	157.28
CAS:	75272-78-5

Physical Properties

Property code	Value	Unit	Source
gf	182.78	kJ/mol	Joback Method
hf	-1.70	kJ/mol	Joback Method
hfus	22.11	kJ/mol	Joback Method
hvap	50.70	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.823		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	2515.07	kPa	Joback Method
rinpol	1427.30		NIST Webbook
rinpol	1427.30		NIST Webbook
tb	553.30	K	Joback Method
tc	757.26	K	Joback Method
tf	279.31	K	Joback Method
vc	0.564	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.00	J/mol×K	553.30	Joback Method
cpg	332.02	J/mol×K	587.29	Joback Method
cpg	343.47	J/mol×K	621.29	Joback Method
cpg	354.35	J/mol×K	655.28	Joback Method
cpg	364.67	J/mol×K	689.27	Joback Method
cpg	374.44	J/mol×K	723.26	Joback Method
cpg	383.67	J/mol×K	757.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75272785&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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