1H-Cyclopenta[b]pyridino-3-carbonitrile, 4,5,6,7-tetrahydro-2-methylthio-4-spirocyclohexar

Inchi: InChI=1S/C15H20N2S/c1-18-14-12(10-16)15(8-3-2-4-9-15)11-6-5-7-13(11)17-14/h7,11,1

InchiKey: OWAKKTNHORDRSL-UHFFFAOYSA-N

Formula: C15H20N2S

SMILES: CSC1=C(C#N)C2(CCCCC2)C2CCC=C2N1

Mol. weight [g/mol]: 260.40

Physical Properties

Property code	Value	Unit	Source
gf	484.43	kJ/mol	Joback Method
hf	195.96	kJ/mol	Joback Method
hfus	27.64	kJ/mol	Joback Method
hvap	75.36	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	3.932		Crippen Method
mcvol	208.740	ml/mol	McGowan Method
pc	2448.32	kPa	Joback Method
rinpol	1337.00		NIST Webbook
rinpol	1337.00		NIST Webbook
tb	821.75	K	Joback Method
tc	1094.11	K	Joback Method
tf	566.67	K	Joback Method
vc	0.794	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.29	J/mol×K	821.75	Joback Method
cpg	651.18	J/mol×K	867.14	Joback Method
cpg	669.56	J/mol×K	912.54	Joback Method
cpg	687.69	J/mol×K	957.93	Joback Method
cpg	705.88	J/mol×K	1003.33	Joback Method
cpg	724.40	J/mol×K	1048.72	Joback Method
cpg	743.54	J/mol×K	1094.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R635068&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