1H-Cyclopenta[b]pyridine-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/h17H,2

InchiKey: YFEFZHHGRHNSPE-UHFFFAOYSA-N

Formula: C15H20N2S

SMILES: CSC1=C(C#N)C2(CCCCC2)C2=C(CCC2)N1

Mol. weight [g/mol]: 260.40

CAS: 309731-99-5

Physical Properties

Property code	Value	Unit	Source
gf	482.51	kJ/mol	Joback Method
hf	204.83	kJ/mol	Joback Method
hfus	26.19	kJ/mol	Joback Method
hvap	76.34	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	4.076		Crippen Method
mcvol	208.740	ml/mol	McGowan Method
pc	2492.52	kPa	Joback Method
rinpol	1337.00		NIST Webbook
rinpol	1337.00		NIST Webbook
tb	831.40	K	Joback Method
tc	1104.04	K	Joback Method
tf	583.43	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.23	J/mol×K	831.40	Joback Method
cpg	645.74	J/mol×K	876.84	Joback Method
cpg	663.87	J/mol×K	922.28	Joback Method
cpg	681.92	J/mol×K	967.72	Joback Method
cpg	700.16	J/mol×K	1013.16	Joback Method
cpg	718.89	J/mol×K	1058.60	Joback Method
cpg	738.39	J/mol×K	1104.04	Joback Method

Sources

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=C309731995&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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