

2-Aminothiazoline

Inchi:	InChI=1S/C3H6N2S/c4-3-5-1-2-6-3/h1-2H2,(H2,4,5)
InchiKey:	REGFWZVTTFGQOJ-UHFFFAOYSA-N
Formula:	C3H6N2S
SMILES:	NC1=NCCS1
Mol. weight [g/mol]:	102.16
CAS:	1779-81-3

Physical Properties

Property code	Value	Unit	Source
hfus	11.21	kJ/mol	Joback Method
ie	8.41	eV	Cheméo Relay (1.0)
logp	0.048		Crippen Method
mcvol	74.280	ml/mol	McGowan Method
tb	490.32	K	Cheméo Relay (1.0)
tf	355.80	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-8.95000e+00
Coeff. B	4.41290e-01
Coeff. C	-2.29300e-04
Coeff. D	3.03000e-08
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):
Joback Method:

https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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