

Cyclohexanone cyanohydrin

Inchi:	InChI=1S/C7H11NO/c8-6-7(9)4-2-1-3-5-7/h9H,1-5H2
InchiKey:	ZDBRPNZOTCHLSP-UHFFFAOYSA-N
Formula:	C7H11NO
SMILES:	N#CC1(O)CCCCC1
Mol. weight [g/mol]:	125.17
CAS:	931-97-5

Physical Properties

Property code	Value	Unit	Source
hfus	5.02	kJ/mol	Joback Method
hvap	69.12	kJ/mol	Cheméo Relay (1.0)
ie	10.31	eV	Cheméo Relay (1.0)
logp	1.205		Crippen Method
mcvol	105.880	ml/mol	McGowan Method
tb	473.13	K	Cheméo Relay (1.0)
tf	308.15	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	-9.67800e+01
Coeff. B	1.05160e+00
Coeff. C	-9.70000e-04
Coeff. D	3.83200e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

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):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization 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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