

Spermidine

Inchi:	InChI=1S/C7H19N3/c8-4-1-2-6-10-7-3-5-9/h10H,1-9H2
InchiKey:	ATHGHQPFPGPMSJY-UHFFFAOYSA-N
Formula:	C7H19N3
SMILES:	NCCCCNCCCN
Mol. weight [g/mol]:	145.25
CAS:	124-20-9

Physical Properties

Property code	Value	Unit	Source
hf	-104.72	kJ/mol	Cheméo Relay (1.0)
hfus	29.38	kJ/mol	Joback Method
hvap	71.98	kJ/mol	Cheméo Relay (1.0)
ie	8.63	eV	Cheméo Relay (1.0)
logp	-0.336		Crippen Method
mcvol	139.430	ml/mol	McGowan Method
pc	3217.33	kPa	Joback Method
tb	517.60	K	Cheméo Relay (1.0)
tc	728.52	K	Cheméo Relay (1.0)
tf	297.15	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	8.29700e+00
Coeff. B	8.68800e-01
Coeff. C	-4.92400e-04
Coeff. D	1.04600e-07
Coeff. E	0.00000e+00
Basis	predicted

Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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