N-(n-Butyl)imidazole

Other names:	1-butyl-1H-imidazole 1-butylimidazole 1-n-butylimidazole 1H-Imidazole, 1-butyl- Butylimidazole Imidazole, 1-butyl- N-Butylimidazole UN 2690
Inchi:	InChI=1S/C7H12N2/c1-2-3-5-9-6-4-8-7-9/h4,6-7H,2-3,5H2,1H3
InchiKey:	MCMFEZDRQOJKMN-UHFFFAOYSA-N
Formula:	C7H12N2
SMILES:	CCCCn1ccnc1
Mol. weight [g/mol]:	124.19

Physical Properties

Property code	Value	Unit	Source
hvap	62.86	kJ/mol	Cheméo Relay (1.0)
ie	8.79	eV	Cheméo Relay (1.0)
logp	1.683		Crippen Method
mcvol	109.990	ml/mol	McGowan Method
rinpol	1164.00		NIST Webbook
rinpol	1164.00		NIST Webbook
ripol	1861.00		NIST Webbook
ripol	1861.00		NIST Webbook
tb	516.82	K	Cheméo Relay (1.0)
tf	223.14	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	63.89	kJ/mol	298.15	Thermochemistry of 1-alkylimidazoles

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Thermochemistry of 1-alkylimidazoles:	https://www.doi.org/10.1016/j.jct.2014.08.020
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4316421&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point