

2-ISOBUTYL-4-METHYLPYRIDINE

Inchi:	InChI=1S/C10H15N/c1-8(2)6-10-7-9(3)4-5-11-10/h4-5,7-8H,6H2,1-3H3
InchiKey:	GZUWMFOJIYTM-TM-UHFFFAOYSA-N
Formula:	C10H15N
SMILES:	<chem>Cc1ccnc(CC(C)C)c1</chem>
Mol. weight [g/mol]:	149.24

Physical Properties

Property code	Value	Unit	Source
hf	-19.74	kJ/mol	Cheméo Relay (1.0)
hvap	53.82	kJ/mol	Cheméo Relay (1.0)
ie	8.90	eV	Cheméo Relay (1.0)
log10ws	-1.47		Cheméo Relay (1.0)
logp	2.589		Crippen Method
mcvol	137.980	ml/mol	McGowan Method
rinpol	1154.00		NIST Webbook
tb	472.79	K	Cheméo Relay (1.0)
tc	684.53	K	Cheméo Relay (1.0)
tf	234.83	K	Cheméo Relay (1.0)

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85665889&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hf: Enthalpy of formation at standard conditions

h_{vap}:	Enthalpy of vaporization at standard conditions
i_e:	Ionization energy
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
ri_{npol}:	Non-polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point

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