2,3,5-TRIMETHYL-6-PROPYLPYRAZINE

Other names: 2-Propyl-3,5,6-trimethylpyrazine
Trimethylpropylpyrazine
Inchi: InChI=1S/C10H16N2/c1-5-6-10-9(4)11-7(2)8(3)12-10/h5-6H2,1-4H3
InchiKey: GEPYSCIASYXPCY-UHFFFAOYSA-N
Formula: C10H16N2
SMILES: CCCc1nc(C)c(C)nc1C
Mol. weight [g/mol]: 164.25

Physical Properties

Property code	Value	Unit	Source
hf	19.53	kJ/mol	Cheméo Relay (1.0)
ie	8.32	eV	Cheméo Relay (1.0)
logp	2.354		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
rinpol	1280.00		NIST Webbook
rinpol	1233.00		NIST Webbook
rinpol	1233.00		NIST Webbook
rinpol	1280.00		NIST Webbook
tb	485.16	K	Cheméo Relay (1.0)
tf	289.34	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C92233824&Units=SI
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

Legend

hf:	Enthalpy of formation at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point