2,3,5-TRIMETHYL-6-BUTYLPYRAZINE

Other names:	2-Butyl-3,5,6-trimethylpyrazine
	Trimethylbutylpyrazine
	Butyltrimethylpyrazine
	Pyrazine, butyltrimethyl-
Inchi:	InChI=1S/C11H18N2/c1-5-6-7-11-10(4)12-8(2)9(3)13-11/h5-7H2,1-4H3
InchiKey:	LHDGCKPZCAXIBB-UHFFFAOYSA-N
Formula:	C11H18N2
SMILES:	CCCCc1nc(C)c(C)nc1C
Mol. weight [g/mol]:	178.28

Physical Properties

Property code	Value	Unit	Source
hf	-3.50	kJ/mol	Cheméo Relay (1.0)
ie	8.30	eV	Cheméo Relay (1.0)
logp	2.744		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
rinpol	1260.00		NIST Webbook
rinpol	1260.00		NIST Webbook
tb	502.13	K	Cheméo Relay (1.0)
tf	284.17	K	Cheméo Relay (1.0)

Sources

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=C10132384&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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