2-METHYL-3-(2-METHYLPROPYL)PYRAZINE

Other names: Pyrazine, 2-methyl-3-(2-methylpropyl)-
2-Methyl-3-(2-methylpropyl)pyrazine
3-Methyl-2-isobutyl pyrazine
Inchi: InChI=1S/C9H14N2/c1-7(2)6-9-8(3)10-4-5-11-9/h4-5,7H,6H2,1-3H3
InchiKey: ZHMIODDNZRIENW-UHFFFAOYSA-N
Formula: C9H14N2
SMILES: Cc1nccnc1CC(C)C
Mol. weight [g/mol]: 150.23

Physical Properties

Property code	Value	Unit	Source
hf	39.78	kJ/mol	Cheméo Relay (1.0)
hvap	58.40	kJ/mol	Cheméo Relay (1.0)
logp	1.984		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
rinpol	1114.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1144.00		NIST Webbook
ripol	1490.00		NIST Webbook
tb	469.47	K	Cheméo Relay (1.0)

Sources

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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13925069&Units=SI

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature