2-METHOXY-3-ETHYLPYRAZINE

Other names: 2-Methoxy-3-ethylpyrazine
Pyrazine, 2-ethyl-3-methoxy-
3-Ethyl-2-methoxypyrazine
Pyrazine, 3-ethyl-2-methoxy
Inchi: InChI=1S/C7H10N2O/c1-3-6-7(10-2)9-5-4-8-6/h4-5H,3H2,1-2H3
InchiKey: DPCILIMHENXHQX-UHFFFAOYSA-N
Formula: C7H10N2O
SMILES: CCc1nccnc1OC
Mol. weight [g/mol]: 138.17

Physical Properties

Property code	Value	Unit	Source
logp	1.048		Crippen Method
mcvol	111.560	ml/mol	McGowan Method
rinpol	1063.00		NIST Webbook
rinpol	1037.00		NIST Webbook
rinpol	1037.00		NIST Webbook
rinpol	1063.00		NIST Webbook
rinpol	1063.00		NIST Webbook
rinpol	1037.00		NIST Webbook
rinpol	1037.00		NIST Webbook
rinpol	1062.00		NIST Webbook
ripol	1400.00		NIST Webbook
ripol	1400.00		NIST Webbook
ripol	1400.00		NIST Webbook
ripol	1400.00		NIST Webbook
tb	457.26	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C25680584&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

Cheméo Relay (1.0):

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature