

Pyrazine, 3-methoxy-2,5-dimethyl-

Other names:	Pyrazine, 3-methoxy-2,5-dimethyl- 2,5-Dimethyl-3-methoxypyrazine
Inchi:	InChI=1S/C7H10N2O/c1-5-4-8-6(2)7(9-5)10-3/h4H,1-3H3
InchiKey:	QYRGVELVPYDICQ-UHFFFAOYSA-N
Formula:	C7H10N2O
SMILES:	COc1nc(C)cnc1C
Mol. weight [g/mol]:	138.17

Physical Properties

Property code	Value	Unit	Source
hf	-69.96	kJ/mol	Cheméo Relay (1.0)
hvap	52.77	kJ/mol	Cheméo Relay (1.0)
logp	1.102		Crippen Method
mcvol	111.560	ml/mol	McGowan Method
rinpol	1054.00		NIST Webbook
rinpol	1065.00		NIST Webbook
rinpol	1057.00		NIST Webbook
ripol	1419.00		NIST Webbook
ripol	1385.00		NIST Webbook
ripol	1421.00		NIST Webbook
tb	458.46	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=C19846221&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
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

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