2,5-DIMETHYL-3-N-PENTYLPYRAZINE

Other names: 2,5-dimethyl-3-pentylpyrazine
Inchi: InChI=1S/C11H18N2/c1-4-5-6-7-11-10(3)12-8-9(2)13-11/h8H,4-7H2,1-3H3
InchiKey: VJNUCPVMBFFSSP-UHFFFAOYSA-N
Formula: C11H18N2
SMILES: CCCCCc1nc(C)cnc1C
Mol. weight [g/mol]: 178.28

Physical Properties

Property code	Value	Unit	Source
hf	-3.62	kJ/mol	Cheméo Relay (1.0)
hvap	65.26	kJ/mol	Cheméo Relay (1.0)
logp	2.826		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
rinpol	1291.00		NIST Webbook
rinpol	1357.00		NIST Webbook
rinpol	1357.00		NIST Webbook
rinpol	1291.00		NIST Webbook
ripol	1680.00		NIST Webbook
tb	511.14	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=C56617697&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
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