2-pentyl-3,5-dimethyl-5,6-dihydropyrazine

Inchi: InChI=1S/C11H20N2/c1-4-5-6-7-11-10(3)13-9(2)8-12-11/h9H,4-8H2,1-3H3
InchiKey: GWJHFKSBVJBUAR-UHFFFAOYSA-N
Formula: C11H20N2
SMILES: CCCCCC1=NCC(C)N=C1C
Mol. weight [g/mol]: 180.29

Physical Properties

Property code	Value	Unit	Source
gf	340.41	kJ/mol	Joback Method
hf	18.51	kJ/mol	Joback Method
hfus	28.02	kJ/mol	Joback Method
hvap	54.84	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	2.871		Crippen Method
mcvol	166.350	ml/mol	McGowan Method
pc	2438.65	kPa	Joback Method
rinpol	1311.00		NIST Webbook
rinpol	1311.00		NIST Webbook
tb	586.31	K	Joback Method
tc	804.58	K	Joback Method
tf	390.75	K	Joback Method
vc	0.654	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.98	J/mol×K	586.31	Joback Method
cpg	470.04	J/mol×K	622.69	Joback Method
cpg	489.03	J/mol×K	659.07	Joback Method
cpg	506.92	J/mol×K	695.44	Joback Method
cpg	523.71	J/mol×K	731.82	Joback Method
cpg	539.39	J/mol×K	768.20	Joback Method
cpg	553.95	J/mol×K	804.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R240987&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume