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

Inchi: InChI=1S/C13H24N2/c1-4-5-6-7-8-9-13-12(3)14-10-11(2)15-13/h11H,4-10H2,1-3H3
InchiKey: VLFBCIPUHLLJEH-UHFFFAOYSA-N
Formula: C13H24N2
SMILES: CCCCCCCC1=NC(C)CN=C1C
Mol. weight [g/mol]: 208.34

Physical Properties

Property code	Value	Unit	Source
gf	357.25	kJ/mol	Joback Method
hf	-22.77	kJ/mol	Joback Method
hfus	33.20	kJ/mol	Joback Method
hvap	59.29	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.651		Crippen Method
mcvol	194.530	ml/mol	McGowan Method
pc	2034.55	kPa	Joback Method
rinpol	1498.00		NIST Webbook
rinpol	1498.00		NIST Webbook
tb	632.07	K	Joback Method
tc	843.07	K	Joback Method
tf	413.29	K	Joback Method
vc	0.766	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.86	J/mol×K	632.07	Joback Method
cpg	576.73	J/mol×K	667.24	Joback Method
cpg	596.43	J/mol×K	702.40	Joback Method
cpg	614.95	J/mol×K	737.57	Joback Method
cpg	632.28	J/mol×K	772.74	Joback Method
cpg	648.44	J/mol×K	807.90	Joback Method
cpg	663.41	J/mol×K	843.07	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R241064&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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