2,3-diethyl-5-methyl-5,6-dihydropyrazine

Inchi: InChI=1S/C9H16N2/c1-4-8-9(5-2)11-7(3)6-10-8/h7H,4-6H2,1-3H3
InchiKey: LTRVKBLOHFHYCL-UHFFFAOYSA-N
Formula: C9H16N2
SMILES: CCC1=NCC(C)N=C1CC
Mol. weight [g/mol]: 152.24

Physical Properties

Property code	Value	Unit	Source
gf	323.57	kJ/mol	Joback Method
hf	59.79	kJ/mol	Joback Method
hfus	22.84	kJ/mol	Joback Method
hvap	50.39	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	2.091		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2976.29	kPa	Joback Method
rinpol	1090.00		NIST Webbook
rinpol	1090.00		NIST Webbook
tb	540.55	K	Joback Method
tc	766.90	K	Joback Method
tf	368.21	K	Joback Method
vc	0.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.35	J/mol×K	540.55	Joback Method
cpg	369.12	J/mol×K	578.28	Joback Method
cpg	386.94	J/mol×K	616.00	Joback Method
cpg	403.77	J/mol×K	653.73	Joback Method
cpg	419.61	J/mol×K	691.45	Joback Method
cpg	434.43	J/mol×K	729.18	Joback Method
cpg	448.21	J/mol×K	766.90	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=R240838&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