3-propyl-2,5-dimethyl-tetrahydropyrazine

Inchi: InChI=1S/C9H18N2/c1-4-5-9-8(3)10-6-7(2)11-9/h7,9,11H,4-6H2,1-3H3
InchiKey: OOGRABCVQSVUNR-UHFFFAOYSA-N
Formula: C9H18N2
SMILES: CCCC1NC(C)CN=C1C
Mol. weight [g/mol]: 154.25

Physical Properties

Property code	Value	Unit	Source
gf	266.46	kJ/mol	Joback Method
hf	-40.02	kJ/mol	Joback Method
hfus	27.53	kJ/mol	Joback Method
hvap	49.67	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	1.608		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	2881.21	kPa	Joback Method
rinpol	1245.00		NIST Webbook
tb	526.59	K	Joback Method
tc	745.40	K	Joback Method
tf	384.18	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.40	J/mol×K	526.59	Joback Method
cpg	370.56	J/mol×K	563.06	Joback Method
cpg	388.81	J/mol×K	599.53	Joback Method
cpg	406.15	J/mol×K	636.00	Joback Method
cpg	422.57	J/mol×K	672.47	Joback Method
cpg	438.06	J/mol×K	708.93	Joback Method
cpg	452.60	J/mol×K	745.40	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R241193&Units=SI

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