Trimethyl-tetrahydropyrazine

Inchi: InChI=1S/C7H16N2/c1-5-4-8-6(2)7(3)9-5/h5-9H,4H2,1-3H3
InchiKey: OMEMBAXECFIRSG-UHFFFAOYSA-N
Formula: C7H16N2
SMILES: CC1CNC(C)C(C)N1
Mol. weight [g/mol]: 128.22

Physical Properties

Property code	Value	Unit	Source
gf	192.51	kJ/mol	Joback Method
hf	-98.55	kJ/mol	Joback Method
hfus	27.04	kJ/mol	Joback Method
hvap	44.50	kJ/mol	Joback Method
log10ws	-1.36		Crippen Method
logp	0.345		Crippen Method
mcvol	118.590	ml/mol	McGowan Method
pc	3456.14	kPa	Joback Method
rinpol	1070.00		NIST Webbook
rinpol	1070.00		NIST Webbook
tb	466.87	K	Joback Method
tc	684.88	K	Joback Method
tf	377.61	K	Joback Method
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.64	J/mol×K	466.87	Joback Method
cpg	277.18	J/mol×K	503.21	Joback Method
cpg	294.01	J/mol×K	539.54	Joback Method
cpg	310.13	J/mol×K	575.88	Joback Method
cpg	325.52	J/mol×K	612.21	Joback Method
cpg	340.17	J/mol×K	648.55	Joback Method
cpg	354.06	J/mol×K	684.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R206427&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

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