2-Pyrazoline, 5-ethyl-4-methyl

Inchi: InChI=1S/C6H12N2/c1-3-6-5(2)4-7-8-6/h4-6,8H,3H2,1-2H3
InchiKey: FANJDTZTMMUBNP-UHFFFAOYSA-N
Formula: C6H12N2
SMILES: CCC1NN=CC1C
Mol. weight [g/mol]: 112.17

Physical Properties

Property code	Value	Unit	Source
gf	262.93	kJ/mol	Joback Method
hf	39.53	kJ/mol	Joback Method
hfus	22.25	kJ/mol	Joback Method
hvap	42.16	kJ/mol	Joback Method
log10ws	-1.44		Crippen Method
logp	0.990		Crippen Method
mcvol	100.200	ml/mol	McGowan Method
pc	3980.54	kPa	Joback Method
rinpol	936.00		NIST Webbook
tb	448.70	K	Joback Method
tc	668.29	K	Joback Method
tf	341.37	K	Joback Method
vc	0.384	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.93	J/mol×K	448.70	Joback Method
cpg	231.30	J/mol×K	485.30	Joback Method
cpg	246.00	J/mol×K	521.90	Joback Method
cpg	260.01	J/mol×K	558.49	Joback Method
cpg	273.34	J/mol×K	595.09	Joback Method
cpg	285.98	J/mol×K	631.69	Joback Method
cpg	297.92	J/mol×K	668.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R511185&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