1-Pyrazoline

Inchi: InChI=1S/C3H6N2/c1-2-4-5-3-1/h1-3H2
InchiKey: DNXIASIHZYFFRO-UHFFFAOYSA-N
Formula: C3H6N2
SMILES: C1CN=NC1
Mol. weight [g/mol]: 70.09
CAS: 2721-43-9

Physical Properties

Property code	Value	Unit	Source
gf	282.16	kJ/mol	Joback Method
hf	175.29	kJ/mol	Joback Method
hfus	7.89	kJ/mol	Joback Method
hvap	35.55	kJ/mol	Joback Method
log10ws	-0.23		Crippen Method
logp	0.842		Crippen Method
mcvol	57.930	ml/mol	McGowan Method
pc	6349.11	kPa	Joback Method
rinpol	697.00		NIST Webbook
rinpol	697.00		NIST Webbook
tb	394.55	K	Joback Method
tc	629.12	K	Joback Method
tf	282.55	K	Joback Method
vc	0.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	109.72	J/mol×K	394.55	Joback Method
cpg	121.96	J/mol×K	433.64	Joback Method
cpg	133.62	J/mol×K	472.74	Joback Method
cpg	144.67	J/mol×K	511.83	Joback Method
cpg	155.12	J/mol×K	550.93	Joback Method
cpg	164.96	J/mol×K	590.02	Joback Method
cpg	174.17	J/mol×K	629.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2721439&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