2-Pyrazoline, 5,5-diethyl

Inchi: InChI=1S/C7H14N2/c1-3-7(4-2)5-6-8-9-7/h6,9H,3-5H2,1-2H3
InchiKey: SUOSNCTVDUSWBT-UHFFFAOYSA-N
Formula: C7H14N2
SMILES: CCC1(CC)CC=NN1
Mol. weight [g/mol]: 126.20

Physical Properties

Property code	Value	Unit	Source
gf	273.57	kJ/mol	Joback Method
hf	54.47	kJ/mol	Joback Method
hfus	17.47	kJ/mol	Joback Method
hvap	43.54	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	1.524		Crippen Method
mcvol	114.290	ml/mol	McGowan Method
pc	3891.64	kPa	Joback Method
rinpol	1005.00		NIST Webbook
rinpol	1005.00		NIST Webbook
tb	476.49	K	Joback Method
tc	702.81	K	Joback Method
tf	380.78	K	Joback Method
vc	0.439	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.53	J/mol×K	476.49	Joback Method
cpg	274.81	J/mol×K	514.21	Joback Method
cpg	290.03	J/mol×K	551.93	Joback Method
cpg	304.29	J/mol×K	589.65	Joback Method
cpg	317.68	J/mol×K	627.37	Joback Method
cpg	330.32	J/mol×K	665.09	Joback Method
cpg	342.30	J/mol×K	702.81	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=R511170&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