2-Pyrazolin-5-one, 3-isobutyl-

Inchi: InChI=1S/C7H12N2O/c1-5(2)3-6-4-7(10)9-8-6/h5H,3-4H2,1-2H3,(H,9,10)
InchiKey: PWHAMHNZTMGTKF-UHFFFAOYSA-N
Formula: C7H12N2O
SMILES: CC(C)CC1=NNC(=O)C1
Mol. weight [g/mol]: 140.18
CAS: 35087-29-7

Physical Properties

Property code	Value	Unit	Source
gf	152.11	kJ/mol	Joback Method
hf	-94.88	kJ/mol	Joback Method
hfus	18.30	kJ/mol	Joback Method
hvap	49.52	kJ/mol	Joback Method
log10ws	-1.52		Crippen Method
logp	0.908		Crippen Method
mcvol	115.860	ml/mol	McGowan Method
pc	3970.51	kPa	Joback Method
tb	553.28	K	Joback Method
tc	792.76	K	Joback Method
tf	426.86	K	Joback Method
vc	0.443	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.22	J/mol×K	553.28	Joback Method
cpg	300.65	J/mol×K	593.19	Joback Method
cpg	315.31	J/mol×K	633.11	Joback Method
cpg	329.17	J/mol×K	673.02	Joback Method
cpg	342.20	J/mol×K	712.93	Joback Method
cpg	354.36	J/mol×K	752.84	Joback Method
cpg	365.62	J/mol×K	792.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35087297&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume