4,4-Dimethyl-5-isopropyl-2-pyrazoline

Inchi: InChI=1S/C8H16N2/c1-6(2)7-8(3,4)5-9-10-7/h5-7,10H,1-4H3
InchiKey: IDMTYGJPXGRQIL-UHFFFAOYSA-N
Formula: C8H16N2
SMILES: CC(C)C1NN=CC1(C)C
Mol. weight [g/mol]: 140.23
CAS: 3674-43-9

Physical Properties

Property code	Value	Unit	Source
gf	271.84	kJ/mol	Joback Method
hf	8.21	kJ/mol	Joback Method
hfus	17.61	kJ/mol	Joback Method
hvap	45.07	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	1.626		Crippen Method
mcvol	128.380	ml/mol	McGowan Method
pc	3364.54	kPa	Joback Method
tb	494.26	K	Joback Method
tc	721.97	K	Joback Method
tf	372.81	K	Joback Method
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.91	J/mol×K	494.26	Joback Method
cpg	322.01	J/mol×K	532.21	Joback Method
cpg	339.00	J/mol×K	570.16	Joback Method
cpg	354.97	J/mol×K	608.11	Joback Method
cpg	370.02	J/mol×K	646.07	Joback Method
cpg	384.26	J/mol×K	684.02	Joback Method
cpg	397.79	J/mol×K	721.97	Joback Method

Sources

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=C3674439&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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