2-Isopropyl-1,3-oxazol-2-ine

Other names: 2-Oxazoline, 2-isopropyl
Inchi: InChI=1S/C6H11NO/c1-5(2)6-7-3-4-8-6/h5H,3-4H2,1-2H3
InchiKey: FVEZUCIZWRDMSJ-UHFFFAOYSA-N
Formula: C6H11NO
SMILES: CC(C)C1=NCCO1
Mol. weight [g/mol]: 113.16
CAS: 10431-99-9

Physical Properties

Property code	Value	Unit	Source
gf	92.45	kJ/mol	Joback Method
hf	-106.35	kJ/mol	Joback Method
hfus	14.59	kJ/mol	Joback Method
hvap	40.80	kJ/mol	Joback Method
log10ws	-0.73		Crippen Method
logp	1.071		Crippen Method
mcvol	96.090	ml/mol	McGowan Method
pc	4109.14	kPa	Joback Method
rinpol	802.00		NIST Webbook
rinpol	802.00		NIST Webbook
tb	440.98	K	Joback Method
tc	659.80	K	Joback Method
tf	268.91	K	Joback Method
vc	0.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.58	J/mol×K	440.98	Joback Method
cpg	218.54	J/mol×K	477.45	Joback Method
cpg	231.78	J/mol×K	513.92	Joback Method
cpg	244.33	J/mol×K	550.39	Joback Method
cpg	256.20	J/mol×K	586.86	Joback Method
cpg	267.38	J/mol×K	623.33	Joback Method

cpg	277.90	J/mol×K	659.80	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=C10431999&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