

N-Isopropylcyclopropanecarboxamide

Other names:	Cyclopropanecarboxamide, N-isopropyl
Inchi:	InChI=1S/C7H13NO/c1-5(2)8-7(9)6-3-4-6/h5-6H,3-4H2,1-2H3,(H,8,9)
InchiKey:	VXCRRRAZVHYGPA-UHFFFAOYSA-N
Formula:	C7H13NO
SMILES:	CC(C)NC(=O)C1CC1
Mol. weight [g/mol]:	127.18
CAS:	26389-62-8

Physical Properties

Property code	Value	Unit	Source
gf	26.84	kJ/mol	Joback Method
hf	-179.40	kJ/mol	Joback Method
hfus	15.20	kJ/mol	Joback Method
hvap	43.88	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	0.921		Crippen Method
mcvol	110.180	ml/mol	McGowan Method
pc	3560.02	kPa	Joback Method
rinpol	1107.00		NIST Webbook
tb	469.90	K	Joback Method
tc	668.97	K	Joback Method
tf	274.18	K	Joback Method
vc	0.419	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.49	J/mol×K	469.90	Joback Method
cpg	257.85	J/mol×K	503.08	Joback Method
cpg	270.43	J/mol×K	536.26	Joback Method
cpg	282.28	J/mol×K	569.43	Joback Method
cpg	293.43	J/mol×K	602.61	Joback Method
cpg	303.92	J/mol×K	635.79	Joback Method
cpg	313.80	J/mol×K	668.97	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C26389628&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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