Carbamic acid, methyl, isopropyl ester

Other names: Isopropyl N-methyl carbamate
Inchi: InChI=1S/C5H11NO2/c1-4(2)8-5(7)6-3/h4H,1-3H3,(H,6,7)
InchiKey: ZLQUUMARLOVRLO-UHFFFAOYSA-N
Formula: C5H11NO2
SMILES: CNC(=O)OC(C)C
Mol. weight [g/mol]: 117.15

Physical Properties

Property code	Value	Unit	Source
gf	-155.75	kJ/mol	Joback Method
hf	-343.14	kJ/mol	Joback Method
hfus	13.07	kJ/mol	Joback Method
hvap	41.93	kJ/mol	Joback Method
log10ws	-1.06		Crippen Method
logp	0.751		Crippen Method
mcvol	98.730	ml/mol	McGowan Method
pc	3759.17	kPa	Joback Method
rinpol	908.00		NIST Webbook
rinpol	908.00		NIST Webbook
ripol	1428.00		NIST Webbook
ripol	1428.00		NIST Webbook
tb	439.82	K	Joback Method
tc	626.93	K	Joback Method
tf	255.93	K	Joback Method
vc	0.368	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.51	J/mol×K	439.82	Joback Method
cpg	211.21	J/mol×K	471.00	Joback Method
cpg	220.57	J/mol×K	502.19	Joback Method
cpg	229.58	J/mol×K	533.37	Joback Method
cpg	238.24	J/mol×K	564.56	Joback Method

cpg	246.55	J/mol×K	595.74	Joback Method
cpg	254.52	J/mol×K	626.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R28031&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume