Carbamic acid, 1-methylethyl ester

Other names:	Carbamic acid, isopropyl ester
	Isopropyl carbamate
	Isopropylester kyseliny karbaminove
Inchi:	InChI=1S/C4H9NO2/c1-3(2)7-4(5)6/h3H,1-2H3,(H2,5,6)
InchiKey:	OVPLZYJGTGDFNB-UHFFFAOYSA-N
Formula:	C4H9NO2
SMILES:	CC(C)OC(N)=O
Mol. weight [g/mol]:	103.12
CAS:	1746-77-6

Physical Properties

Property code	Value	Unit	Source
gf	-187.11	kJ/mol	Joback Method
hf	-342.18	kJ/mol	Joback Method
hfus	10.58	kJ/mol	Joback Method
hvap	43.91	kJ/mol	Joback Method
log10ws	-0.88		Crippen Method
logp	0.490		Crippen Method
mcvol	84.640	ml/mol	McGowan Method
pc	4498.26	kPa	Joback Method
tb	439.30	K	Joback Method
tc	638.45	K	Joback Method
tf	275.26	K	Joback Method
vc	0.306	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.46	J/mol×K	439.30	Joback Method
cpg	180.72	J/mol×K	472.49	Joback Method
cpg	188.69	J/mol×K	505.68	Joback Method
cpg	196.36	J/mol×K	538.88	Joback Method
cpg	203.72	J/mol×K	572.07	Joback Method
cpg	210.77	J/mol×K	605.26	Joback Method

cpg	217.51	J/mol×K	638.45	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	454.20	K	94.80	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1746776&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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