

Carbamic acid, vinyl-, tert-butyl ester

Inchi:	InChI=1S/C7H13NO2/c1-5-8-6(9)10-7(2,3)4/h5H,1H2,2-4H3,(H,8,9)
InchiKey:	SJDWKAHMQWSMPV-UHFFFAOYSA-N
Formula:	C7H13NO2
SMILES:	C=CNC(=O)OC(C)(C)C
Mol. weight [g/mol]:	143.18
CAS:	7150-72-3

Physical Properties

Property code	Value	Unit	Source
gf	-45.79	kJ/mol	Joback Method
hf	-262.46	kJ/mol	Joback Method
hfus	13.08	kJ/mol	Joback Method
hvap	44.80	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	1.655		Crippen Method
mcvol	122.610	ml/mol	McGowan Method
pc	3191.93	kPa	Joback Method
tb	479.47	K	Joback Method
tc	674.19	K	Joback Method
tf	294.13	K	Joback Method
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.67	J/mol×K	479.47	Joback Method
cpg	280.77	J/mol×K	511.92	Joback Method
cpg	292.22	J/mol×K	544.38	Joback Method
cpg	303.06	J/mol×K	576.83	Joback Method
cpg	313.30	J/mol×K	609.28	Joback Method
cpg	322.96	J/mol×K	641.74	Joback Method
cpg	332.08	J/mol×K	674.19	Joback Method

Sources

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=C7150723&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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