carbamic acid

Inchi: InChI=1S/C6H13NO2/c1-6(2,3)4-9-5(7)8/h4H2,1-3H3,(H2,7,8)
InchiKey: AFQYFVWMIRMBAE-UHFFFAOYSA-N
Formula: C6H13NO2
SMILES: CC(C)(C)COC(N)=O
Mol. weight [g/mol]: 131.17

Physical Properties

Property code	Value	Unit	Source
gf	-164.99	kJ/mol	Joback Method
hf	-386.93	kJ/mol	Joback Method
hfus	11.87	kJ/mol	Joback Method
hvap	47.45	kJ/mol	Joback Method
log10ws	-0.80		Aqueous Solubility Prediction Method
logp	1.128		Crippen Method
mcvol	112.820	ml/mol	McGowan Method
pc	3577.07	kPa	Joback Method
tb	482.27	K	Joback Method
tc	684.80	K	Joback Method
tf	315.22	K	Joback Method
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.23	J/mol×K	482.27	Joback Method
cpg	265.78	J/mol×K	516.03	Joback Method
cpg	276.73	J/mol×K	549.78	Joback Method
cpg	287.09	J/mol×K	583.54	Joback Method
cpg	296.88	J/mol×K	617.29	Joback Method
cpg	306.12	J/mol×K	651.05	Joback Method
cpg	314.83	J/mol×K	684.80	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

https://www.chemeo.com/cid/103-707-2/carbamic-acid.pdf

Generated by Cheméo on 2024-10-12 08:11:13.227191713 +0000 UTC m=+3301535.864160972.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.