Carbamic acid, phenyl ester

Other names: Phenyl carbamate
Inchi: InChI=1S/C7H7NO2/c8-7(9)10-6-4-2-1-3-5-6/h1-5H,(H2,8,9)
InchiKey: BSCCSDNZEIHXOK-UHFFFAOYSA-N
Formula: C7H7NO2
SMILES: NC(=O)Oc1ccccc1
Mol. weight [g/mol]: 137.14
CAS: 622-46-8

Physical Properties

Property code	Value	Unit	Source
gf	-47.00	kJ/mol	Joback Method
hf	-162.29	kJ/mol	Joback Method
hfus	15.91	kJ/mol	Joback Method
hvap	53.25	kJ/mol	Joback Method
ie	9.14	eV	NIST Webbook
log10ws	-1.78		Crippen Method
logp	1.144		Crippen Method
mcvol	103.150	ml/mol	McGowan Method
pc	4717.12	kPa	Joback Method
ripol	2006.00		NIST Webbook
ripol	2006.00		NIST Webbook
ripol	2006.00		NIST Webbook
tb	535.06	K	Joback Method
tc	769.17	K	Joback Method
tf	350.49	K	Joback Method
vc	0.372	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.35	J/mol×K	535.06	Joback Method
cpg	232.77	J/mol×K	574.08	Joback Method
cpg	242.51	J/mol×K	613.10	Joback Method
cpg	251.57	J/mol×K	652.12	Joback Method

cpg	259.99	J/mol×K	691.13	Joback Method
cpg	267.77	J/mol×K	730.15	Joback Method
cpg	274.92	J/mol×K	769.17	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C622468&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume