Cyanic acid, phenyl ester

Other names: Phenyl cyanate
Inchi: InChI=1S/C7H5NO/c8-6-9-7-4-2-1-3-5-7/h1-5H
InchiKey: CWHFDTWZHFRTAB-UHFFFAOYSA-N
Formula: C7H5NO
SMILES: N#COc1ccccc1
Mol. weight [g/mol]: 119.12
CAS: 1122-85-6

Physical Properties

Property code	Value	Unit	Source
chl	-3557.00 ± 0.80	kJ/mol	NIST Webbook
gf	148.65	kJ/mol	Joback Method
hf	81.38	kJ/mol	Joback Method
hfl	88.30 ± 0.80	kJ/mol	NIST Webbook
hfus	10.62	kJ/mol	Joback Method
hvap	46.34	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	1.546		Crippen Method
mcvol	92.980	ml/mol	McGowan Method
pc	3901.37	kPa	Joback Method
tb	510.74	K	Joback Method
tc	743.84	K	Joback Method
tf	282.29	K	Joback Method
vc	0.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	181.47	J/mol×K	510.74	Joback Method
cpg	190.45	J/mol×K	549.59	Joback Method
cpg	198.87	J/mol×K	588.44	Joback Method
cpg	206.75	J/mol×K	627.29	Joback Method
cpg	214.08	J/mol×K	666.14	Joback Method
cpg	220.90	J/mol×K	704.99	Joback Method

cpg	227.20	J/mol×K	743.84	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=C1122856&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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