L-Homoserine lactone, N-pentafluoropropionyl-

Inchi: InChI=1S/C7H6F5NO3/c8-6(9,7(10,11)12)5(15)13-3-1-2-16-4(3)14/h3H,1-2H2,(H,13,15)

InchiKey: RNSQINXUQVPRPY-UHFFFAOYSA-N

Formula: C7H6F5NO3

SMILES: O=C1OCCC1NC(=O)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 247.12

Physical Properties

Property code	Value	Unit	Source
gf	-1172.00	kJ/mol	Joback Method
hf	-1454.19	kJ/mol	Joback Method
hfus	22.58	kJ/mol	Joback Method
hvap	46.70	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	0.616		Crippen Method
mcvol	126.470	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
rinpol	1186.00		NIST Webbook
tb	563.54	K	Joback Method
tc	760.72	K	Joback Method
tf	384.72	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.84	J/mol×K	563.54	Joback Method
cpg	358.72	J/mol×K	596.40	Joback Method
cpg	369.77	J/mol×K	629.27	Joback Method
cpg	380.00	J/mol×K	662.13	Joback Method
cpg	389.46	J/mol×K	694.99	Joback Method
cpg	398.18	J/mol×K	727.86	Joback Method
cpg	406.20	J/mol×K	760.72	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=U374762&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume