

Hydroxylamine, O-pentafluorobenzoyl

Inchi: InChI=1S/C6H2F5NO/c7-1-2(8)4(10)6(13-12)5(11)3(1)9/h12H2
InchiKey: AUPSECUITDVBHD-UHFFFAOYSA-N
Formula: C6H2F5NO
SMILES: NOc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 199.08

Physical Properties

Property code	Value	Unit	Source
gf	-948.70	kJ/mol	Joback Method
hf	-1066.97	kJ/mol	Joback Method
hfus	25.18	kJ/mol	Joback Method
hvap	43.50	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	1.635		Crippen Method
mcvol	96.340	ml/mol	McGowan Method
pc	3368.44	kPa	Joback Method
rinpol	1068.00		NIST Webbook
rinpol	1068.00		NIST Webbook
tb	479.56	K	Joback Method
tc	659.87	K	Joback Method
tf	354.84	K	Joback Method
vc	0.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	210.79	J/molxK	479.56	Joback Method
cpg	216.87	J/molxK	509.61	Joback Method
cpg	222.77	J/molxK	539.66	Joback Method
cpg	228.49	J/molxK	569.72	Joback Method
cpg	234.01	J/molxK	599.77	Joback Method
cpg	239.34	J/molxK	629.82	Joback Method
cpg	244.45	J/molxK	659.87	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R333143&Units=SI

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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