

N-Hydroxypentafluoro benzamide

Inchi:	InChI=1S/C7H2F5NO2/c8-2-1(7(14)13-15)3(9)5(11)6(12)4(2)10/h15H,(H,13,14)
InchiKey:	MANBOMDQSIJBG-UHFFFAOYSA-N
Formula:	C7H2F5NO2
SMILES:	O=C(NO)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	227.09
CAS:	80684-62-4

Physical Properties

Property code	Value	Unit	Source
gf	-1078.08	kJ/mol	Joback Method
hf	-1200.52	kJ/mol	Joback Method
hfus	32.17	kJ/mol	Joback Method
hvap	62.54	kJ/mol	Joback Method
ie	10.20	eV	NIST Webbook
log10ws	-2.71		Crippen Method
logp	1.501		Crippen Method
mcvol	112.000	ml/mol	McGowan Method
pc	3497.14	kPa	Joback Method
tb	603.71	K	Joback Method
tc	777.01	K	Joback Method
tf	424.03	K	Joback Method
vc	0.469	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.32	J/mol×K	603.71	Joback Method
cpg	275.28	J/mol×K	632.59	Joback Method
cpg	280.95	J/mol×K	661.48	Joback Method
cpg	286.34	J/mol×K	690.36	Joback Method
cpg	291.44	J/mol×K	719.24	Joback Method
cpg	296.26	J/mol×K	748.13	Joback Method
cpg	300.81	J/mol×K	777.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80684624&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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