Benzamide, 2,3,4,5,6-pentafluoro-

Other names:	2,3,4,5,6-Pentafluorobenzamide
	Pentafluorobenzamide
	Benzamide, pentafluoro-
Inchi:	InChI=1S/C7H2F5NO/c8-2-1(7(13)14)3(9)5(11)6(12)4(2)10/h(H2,13,14)
InchiKey:	WPWWHXPRJFDTTJ-UHFFFAOYSA-N
Formula:	C7H2F5NO
SMILES:	NC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	211.09
CAS:	652-31-3

Physical Properties

Property code	Value	Unit	Source
gf	-964.20	kJ/mol	Joback Method
hf	-1067.97	kJ/mol	Joback Method
hfus	28.18	kJ/mol	Joback Method
hvap	50.06	kJ/mol	Joback Method
ie	10.00	eV	NIST Webbook
ie	10.00 ± 0.10	eV	NIST Webbook
log10ws	-3.30		Crippen Method
logp	1.481		Crippen Method
mcvol	106.130	ml/mol	McGowan Method
pc	3306.75	kPa	Joback Method
tb	533.89	K	Joback Method
tc	722.43	K	Joback Method
tf	393.81	K	Joback Method
vc	0.445	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.07	J/mol×K	533.89	Joback Method
cpg	245.75	J/mol×K	565.31	Joback Method
cpg	252.12	J/mol×K	596.74	Joback Method
cpg	258.19	J/mol×K	628.16	Joback Method

cpg	263.96	J/mol×K	659.58	Joback Method
cpg	269.42	J/mol×K	691.01	Joback Method
cpg	274.58	J/mol×K	722.43	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=C652313&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
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