

Methanone, bis(pentafluorophenyl)-

Other names:	Benzophenone, decafluoro- Decafluorobenzophenone Perfluorobenzophenone
Inchi:	InChI=1S/C13F10O/c14-3-1(4(15)8(19)11(22)7(3)18)13(24)2-5(16)9(20)12(23)10(21)6(2
InchiKey:	WWQLXRAKBJVNCC-UHFFFAOYSA-N
Formula:	C13F10O
SMILES:	O=C(c1c(F)c(F)c(F)c1F)c1c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	362.12
CAS:	853-39-4

Physical Properties

Property code	Value	Unit	Source
ea	1.52 ± 0.11	eV	NIST Webbook
gf	-1889.92	kJ/mol	Joback Method
hf	-2026.97	kJ/mol	Joback Method
hfus	46.02	kJ/mol	Joback Method
hvap	54.28	kJ/mol	Joback Method
ie	10.15	eV	NIST Webbook
log10ws	-6.75		Crippen Method
logp	4.309		Crippen Method
mcvol	165.780	ml/mol	McGowan Method
pc	1824.72	kPa	Joback Method
tb	646.57	K	Joback Method
tc	817.83	K	Joback Method
tf	470.14	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.64	J/mol×K	646.57	Joback Method
cpg	420.47	J/mol×K	675.11	Joback Method
cpg	427.92	J/mol×K	703.66	Joback Method
cpg	434.99	J/mol×K	732.20	Joback Method

cpg	441.66	J/mol×K	760.74	Joback Method
cpg	447.95	J/mol×K	789.28	Joback Method
cpg	453.85	J/mol×K	817.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C853394&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
ea:	Electron affinity
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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