

Methanone, (pentafluorophenyl)phenyl-

Other names:	Benzophenone, 2,3,4,5,6-pentafluoro- Benzoylpentafluorobenzene 2,3,4,5,6-Pentafluorobenzophenone Pentafluorobenzophenone
Inchi:	InChI=1S/C13H5F5O/c14-8-7(9(15)11(17)12(18)10(8)16)13(19)6-4-2-1-3-5-6/h1-5H
InchiKey:	HCCPWOWOSASKLG-UHFFFAOYSA-N
Formula:	C13H5F5O
SMILES:	O=C(c1ccccc1)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	272.17
CAS:	1536-23-8

Physical Properties

Property code	Value	Unit	Source
gf	-867.72	kJ/mol	Joback Method
hf	-989.07	kJ/mol	Joback Method
hfus	32.56	kJ/mol	Joback Method
hvap	55.05	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	3.613		Crippen Method
mcvol	156.930	ml/mol	McGowan Method
pc	2400.57	kPa	Joback Method
tb	625.32	K	Joback Method
tc	827.85	K	Joback Method
tf	404.59	K	Joback Method
vc	0.643	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.34	J/molxK	625.32	Joback Method
cpg	389.00	J/molxK	659.08	Joback Method
cpg	398.99	J/molxK	692.83	Joback Method
cpg	408.31	J/molxK	726.59	Joback Method
cpg	417.00	J/molxK	760.34	Joback Method

cpg	425.07	J/mol×K	794.10	Joback Method
cpg	432.55	J/mol×K	827.85	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	366.20	K	0.03	NIST Webbook
tbrp	366.00	K	0.03	NIST Webbook

Sources

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=C1536238&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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