

Pentafluorobenzoyl chloride

Other names:	2,3,4,5,6-Pentafluorobenzoyl chloride Benzoyl chloride, pentafluoro- Pentafluorobenzyl chloride
Inchi:	InChI=1S/C7ClF5O/c8-7(14)1-2(9)4(11)6(13)5(12)3(1)10
InchiKey:	MYHOHFDYWMPGJY-UHFFFAOYSA-N
Formula:	C7ClF5O
SMILES:	O=C(Cl)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	230.52
CAS:	2251-50-5

Physical Properties

Property code	Value	Unit	Source
gf	-1042.58	kJ/mol	Joback Method
hf	-1117.50	kJ/mol	Joback Method
hfus	27.18	kJ/mol	Joback Method
hvap	43.81	kJ/mol	Joback Method
ie	9.80	eV	NIST Webbook
ie	10.20	eV	NIST Webbook
log10ws	-4.02		Crippen Method
logp	2.761		Crippen Method
mcvol	108.390	ml/mol	McGowan Method
pc	2976.29	kPa	Joback Method
rinpola	922.00		NIST Webbook
rinpola	922.00		NIST Webbook
tb	431.50 ± 0.50	K	NIST Webbook
tb	431.70	K	NIST Webbook
tc	682.22	K	Joback Method
tf	340.47	K	Joback Method
vc	0.465	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.64	J/mol×K	498.79	Joback Method

cpg	221.47	J/mol×K	529.36	Joback Method
cpg	227.04	J/mol×K	559.93	Joback Method
cpg	232.36	J/mol×K	590.50	Joback Method
cpg	237.42	J/mol×K	621.07	Joback Method
cpg	242.24	J/mol×K	651.64	Joback Method
cpg	246.80	J/mol×K	682.22	Joback Method

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=C2251505&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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