Pentafluorobenzaldehyde

Other names: 2,3,4,5,6-Pentafluorobenzaldehyde
Benzaldehyde, pentafluoro-
Benzaldehyde, 2,3,4,5,6-pentafluoro-
Inchi: InChI=1S/C7HF5O/c8-3-2(1-13)4(9)6(11)7(12)5(3)10/h1H
InchiKey: QJXCFMJTJYCLFG-UHFFFAOYSA-N
Formula: C7HF5O
SMILES: O=Cc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 196.07
CAS: 653-37-2

Physical Properties

Property code	Value	Unit	Source
ea	1.10 ± 0.11	eV	NIST Webbook
gf	-1001.25	kJ/mol	Joback Method
hf	-1074.76	kJ/mol	Joback Method
hfus	23.67	kJ/mol	Joback Method
hvap	39.40	kJ/mol	Joback Method
ie	10.35	eV	NIST Webbook
log10ws	-3.37		Crippen Method
logp	2.195		Crippen Method
mcvol	96.150	ml/mol	McGowan Method
pc	3138.51	kPa	Joback Method
rinpol	943.00		NIST Webbook
rinpol	943.00		NIST Webbook
tb	438.00 ± 1.00	K	NIST Webbook
tb	438.20	K	NIST Webbook
tb	438.00 ± 1.00	K	NIST Webbook
tc	629.33	K	Joback Method
tf	302.62	K	Joback Method
vc	0.426	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	197.90	J/mol×K	456.15	Joback Method
cpg	203.81	J/mol×K	485.01	Joback Method
cpg	209.51	J/mol×K	513.88	Joback Method
cpg	214.98	J/mol×K	542.74	Joback Method
cpg	220.25	J/mol×K	571.61	Joback Method
cpg	225.29	J/mol×K	600.47	Joback Method
cpg	230.12	J/mol×K	629.33	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C653372&Units=SI

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
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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