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

Physical Properties

Property code	Value	Unit	Source
ea	1.10 ± 0.11	eV	NIST Webbook
hfus	23.67	kJ/mol	Joback Method
ie	10.35	eV	NIST Webbook
logp	2.195		Crippen Method
mcvol	96.150	ml/mol	McGowan Method
rinpol	943.00		NIST Webbook
rinpol	943.00		NIST Webbook
tb	438.00 ± 1.00	K	NIST Webbook
tb	438.00 ± 1.00	K	NIST Webbook
tb	438.20	K	NIST Webbook

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:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C653372&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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