

2,4-DIFLUOROBENZALDEHYDE

Other names:	Benzaldehyde, 2,4-difluoro-
Inchi:	InChI=1S/C7H4F2O/c8-6-2-1-5(4-10)7(9)3-6/h1-4H
InchiKey:	WCGPCBACLBHDCI-UHFFFAOYSA-N
Formula:	C7H4F2O
SMILES:	O=Cc1ccc(F)cc1F
Mol. weight [g/mol]:	142.10

Physical Properties

Property code	Value	Unit	Source
hfus	15.60	kJ/mol	Joback Method
hvap	53.92	kJ/mol	Cheméo Relay (1.0)
ie	9.65	eV	Cheméo Relay (1.0)
logp	1.777		Crippen Method
mcvol	90.840	ml/mol	McGowan Method
tb	444.68	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.68	J/mol×K	443.40	Joback Method
cpg	180.87	J/mol×K	476.47	Joback Method
cpg	188.63	J/mol×K	509.54	Joback Method
cpg	195.96	J/mol×K	542.61	Joback Method
cpg	202.88	J/mol×K	575.68	Joback Method
cpg	209.41	J/mol×K	608.75	Joback Method
cpg	215.55	J/mol×K	641.82	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	338.70	K	2.30	NIST Webbook

Sources

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
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=C1550352&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

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