2,6-Difluorobenzaldehyde

Other names: Benzaldehyde, 2,6-difluoro-
Inchi: InChI=1S/C7H4F2O/c8-6-2-1-3-7(9)5(6)4-10/h1-4H
InchiKey: SOWRUJSGHKNOKN-UHFFFAOYSA-N
Formula: C7H4F2O
SMILES: O=Cc1c(F)cccc1F
Mol. weight [g/mol]: 142.10
CAS: 437-81-0

Physical Properties

Property code	Value	Unit	Source
gf	-387.93	kJ/mol	Joback Method
hf	-452.02	kJ/mol	Joback Method
hfus	15.60	kJ/mol	Joback Method
hvap	39.86	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	1.777		Crippen Method
mcvol	90.840	ml/mol	McGowan Method
pc	3881.95	kPa	Joback Method
tb	443.40	K	Joback Method
tc	641.82	K	Joback Method
tf	263.29	K	Joback Method
vc	0.372	m3/kmol	Joback Method

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	356.20	K	2.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C437810&Units=SI
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

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