

4-Fluoro-2-nitrobenzaldehyde

Inchi:	InChI=1S/C7H4FNO3/c8-6-2-1-5(4-10)7(3-6)9(11)12/h1-4H
InchiKey:	ORCGMGUNVGVHDN-UHFFFAOYSA-N
Formula:	C7H4FNO3
SMILES:	O=Cc1ccc(F)cc1[N+](=O)[O-]
Mol. weight [g/mol]:	169.11
CAS:	2923-96-8

Physical Properties

Property code	Value	Unit	Source
gf	-157.57	kJ/mol	Joback Method
hf	-266.67	kJ/mol	Joback Method
hfus	23.88	kJ/mol	Joback Method
hvap	57.27	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	1.546		Crippen Method
mcvol	106.490	ml/mol	McGowan Method
pc	4173.09	kPa	Joback Method
tb	595.97	K	Joback Method
tc	835.95	K	Joback Method
tf	406.31	K	Joback Method
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.50	J/molxK	595.97	Joback Method
cpg	248.15	J/molxK	635.97	Joback Method
cpg	256.14	J/molxK	675.96	Joback Method
cpg	263.50	J/molxK	715.96	Joback Method
cpg	270.25	J/molxK	755.95	Joback Method
cpg	276.43	J/molxK	795.95	Joback Method
cpg	282.05	J/molxK	835.95	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=C2923968&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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