2,5-DIFLUOROBENZALDEHYDE

Inchi: InChI=1S/C7H4F2O/c8-6-1-2-7(9)5(3-6)4-10/h1-4H
InchiKey: VVVOJODFBWBNBI-UHFFFAOYSA-N
Formula: C7H4F2O
SMILES: O=Cc1cc(F)ccc1F
Mol. weight [g/mol]: 142.10

Physical Properties

Property code	Value	Unit	Source
hfus	15.60	kJ/mol	Joback Method
hvap	53.76	kJ/mol	Cheméo Relay (1.0)
ie	9.58	eV	Cheméo Relay (1.0)
logp	1.777		Crippen Method
mcvol	90.840	ml/mol	McGowan Method
tb	445.76	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	341.20	K	2.30	NIST Webbook

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=C2646904&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
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