3-F-4-CH3O-C6H3-CCH

Inchi: InChI=1S/C9H7FO/c1-3-7-4-5-9(11-2)8(10)6-7/h1,4-6H,2H3
InchiKey: PCQZNIONNPEWAZ-UHFFFAOYSA-N
Formula: C9H7FO
SMILES: C#Cc1ccc(OC)c(F)c1
Mol. weight [g/mol]: 150.15
CAS: 120136-28-9

Physical Properties

Property code	Value	Unit	Source
affp	871.90	kJ/mol	NIST Webbook
basg	839.50	kJ/mol	NIST Webbook
gf	41.31	kJ/mol	Joback Method
hf	-51.93	kJ/mol	Joback Method
hfus	19.57	kJ/mol	Joback Method
hvap	40.68	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	1.816		Crippen Method
mcvol	112.950	ml/mol	McGowan Method
pc	3480.65	kPa	Joback Method
tb	453.77	K	Joback Method
tc	666.17	K	Joback Method
tf	312.44	K	Joback Method
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.14	J/mol×K	453.77	Joback Method
cpg	228.54	J/mol×K	489.17	Joback Method
cpg	238.42	J/mol×K	524.57	Joback Method
cpg	247.80	J/mol×K	559.97	Joback Method
cpg	256.70	J/mol×K	595.37	Joback Method
cpg	265.11	J/mol×K	630.77	Joback Method
cpg	273.05	J/mol×K	666.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C120136289&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

affp:	Proton affinity
basg:	Gas basicity
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume