3-FC6H4C(CH3)=CH2

Inchi: InChI=1S/C9H9F/c1-7(2)8-4-3-5-9(10)6-8/h3-6H,1H2,2H3
InchiKey: RSKZYVKOUASPDU-UHFFFAOYSA-N
Formula: C9H9F
SMILES: C=C(C)c1cccc(F)c1
Mol. weight [g/mol]: 136.17
CAS: 3825-81-8

Physical Properties

Property code	Value	Unit	Source
affp	839.70	kJ/mol	NIST Webbook
basg	810.80	kJ/mol	NIST Webbook
gf	12.16	kJ/mol	Joback Method
hf	-84.50	kJ/mol	Joback Method
hfus	13.21	kJ/mol	Joback Method
hvap	37.16	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.859		Crippen Method
mcvol	111.380	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
tb	432.81	K	Joback Method
tc	638.60	K	Joback Method
tf	215.00	K	Joback Method
vc	0.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.22	J/mol×K	432.81	Joback Method
cpg	220.62	J/mol×K	467.11	Joback Method
cpg	232.31	J/mol×K	501.41	Joback Method
cpg	243.32	J/mol×K	535.70	Joback Method
cpg	253.67	J/mol×K	570.00	Joback Method
cpg	263.41	J/mol×K	604.30	Joback Method
cpg	272.55	J/mol×K	638.60	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3825818&Units=SI

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