3-CF3C6H4C(CH3)=CH2

Inchi: InChI=1S/C10H9F3/c1-7(2)8-4-3-5-9(6-8)10(11,12)13/h3-6H,1H2,2H3
InchiKey: GLLSGNKQMPAEQV-UHFFFAOYSA-N
Formula: C10H9F3
SMILES: C=C(C)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 186.17
CAS: 368-79-6

Physical Properties

Property code	Value	Unit	Source
affp	823.70	kJ/mol	NIST Webbook
basg	794.80	kJ/mol	NIST Webbook
gf	-366.20	kJ/mol	Joback Method
hf	-506.11	kJ/mol	Joback Method
hfus	14.54	kJ/mol	Joback Method
hvap	36.45	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.739		Crippen Method
mcvol	129.010	ml/mol	McGowan Method
pc	2681.86	kPa	Joback Method
tb	451.00	K	Joback Method
tc	645.70	K	Joback Method
tf	229.87	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.95	J/mol×K	451.00	Joback Method
cpg	281.43	J/mol×K	483.45	Joback Method
cpg	294.04	J/mol×K	515.90	Joback Method
cpg	305.81	J/mol×K	548.35	Joback Method
cpg	316.79	J/mol×K	580.80	Joback Method
cpg	327.03	J/mol×K	613.25	Joback Method
cpg	336.57	J/mol×K	645.70	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=C368796&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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