«alpha»-Fluorocinnamic acid

Other names: 2-Propenoic acid, 2-fluoro-3-phenyl-
Cinnamic acid, «alpha»-fluoro-
alpha-Fluorocinnamic acid
Inchi: InChI=1S/C9H7FO2/c10-8(9(11)12)6-7-4-2-1-3-5-7/h1-6H,(H,11,12)/b8-6-
InchiKey: QONCEXMULRJPPY-VURMDHGXSA-N
Formula: C9H7FO2
SMILES: O=C(O)C(F)=Cc1ccccc1
Mol. weight [g/mol]: 166.15
CAS: 350-90-3

Physical Properties

Property code	Value	Unit	Source
chs	-4240.69	kJ/mol	NIST Webbook
gf	-251.57	kJ/mol	Joback Method
hf	-346.05	kJ/mol	Joback Method
hfus	20.77	kJ/mol	Joback Method
hvap	60.55	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.082		Crippen Method
mcvol	118.820	ml/mol	McGowan Method
pc	3985.56	kPa	Joback Method
tb	563.20	K	NIST Webbook
tc	786.96	K	Joback Method
tf	309.91	K	Joback Method
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.19	J/mol×K	581.36	Joback Method
cpg	278.65	J/mol×K	615.63	Joback Method
cpg	287.45	J/mol×K	649.89	Joback Method
cpg	295.62	J/mol×K	684.16	Joback Method
cpg	303.21	J/mol×K	718.43	Joback Method

cpg	310.26	J/mol×K	752.69	Joback Method
cpg	316.81	J/mol×K	786.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C350903&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

chs:	Standard solid enthalpy of combustion
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