

2-Propenoic acid, 3-(2-fluorophenyl)-

Other names:	Cinnamic acid, o-fluoro- o-Fluorocinnamic acid 3-(2-Fluorophenyl)propenoic acid 2-Fluorocinnamic acid 3-(2-Fluoro-phenyl)-acrylic acid 3-(2-Fluorophenyl)-2-propenoic acid
Inchi:	InChI=1S/C9H7FO2/c10-8-4-2-1-3-7(8)5-6-9(11)12/h1-6H,(H,11,12)/b6-5+
InchiKey:	IOUDZAFBPDDAMK-AATRIKPKSA-N
Formula:	C9H7FO2
SMILES:	O=C(O)C=Cc1ccccc1F
Mol. weight [g/mol]:	166.15
CAS:	451-69-4

Physical Properties

Property code	Value	Unit	Source
gf	-252.65	kJ/mol	Joback Method
hf	-347.73	kJ/mol	Joback Method
hfus	21.69	kJ/mol	Joback Method
hvap	61.13	kJ/mol	Joback Method
ie	9.00	eV	NIST Webbook
log10ws	-2.14		Crippen Method
logp	1.924		Crippen Method
mcvol	118.820	ml/mol	McGowan Method
pc	3886.79	kPa	Joback Method
tb	586.46	K	Joback Method
tc	789.56	K	Joback Method
tf	336.39	K	Joback Method
vc	0.455	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.26	J/molxK	586.46	Joback Method
cpg	277.34	J/molxK	620.31	Joback Method

cpg	285.83	J/mol×K	654.16	Joback Method
cpg	293.75	J/mol×K	688.01	Joback Method
cpg	301.14	J/mol×K	721.86	Joback Method
cpg	308.03	J/mol×K	755.71	Joback Method
cpg	314.47	J/mol×K	789.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C451694&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Legend

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
hvac:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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