2,5-Difluorocinnamic acid

Inchi: InChI=1S/C9H6F2O2/c10-7-2-3-8(11)6(5-7)1-4-9(12)13/h1-5H,(H,12,13)/b4-1+
InchiKey: XAWHCSKPALFWBI-DAFODLJHSA-N
Formula: C9H6F2O2
SMILES: O=C(O)C=Cc1cc(F)ccc1F
Mol. weight [g/mol]: 184.14
CAS: 112898-33-6

Physical Properties

Property code	Value	Unit	Source
gf	-457.09	kJ/mol	Joback Method
hf	-555.31	kJ/mol	Joback Method
hfus	24.38	kJ/mol	Joback Method
hvap	60.98	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.063		Crippen Method
mcvol	120.590	ml/mol	McGowan Method
pc	3611.55	kPa	Joback Method
tb	590.71	K	Joback Method
tc	785.69	K	Joback Method
tf	349.50	K	Joback Method
vc	0.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.34	J/mol×K	590.71	Joback Method
cpg	283.75	J/mol×K	623.21	Joback Method
cpg	291.65	J/mol×K	655.70	Joback Method
cpg	299.05	J/mol×K	688.20	Joback Method
cpg	305.99	J/mol×K	720.70	Joback Method
cpg	312.48	J/mol×K	753.20	Joback Method
cpg	318.57	J/mol×K	785.69	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=C112898336&Units=SI

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
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