2,3,4,5,6-Pentafluorocinnamic acid

Other names: Pentafluorocinnamic acid
Inchi: InChI=1S/C9H3F5O2/c10-5-3(1-2-4(15)16)6(11)8(13)9(14)7(5)12/h1-2H,(H,15,16)/b2-1+
InchiKey: IUUKDBLGVZISGW-OWOJBTEDSA-N
Formula: C9H3F5O2
SMILES: O=C(O)C=Cc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 238.11
CAS: 719-60-8

Physical Properties

Property code	Value	Unit	Source
gf	-1070.41	kJ/mol	Joback Method
hf	-1178.05	kJ/mol	Joback Method
hfus	32.45	kJ/mol	Joback Method
hvap	60.51	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	2.480		Crippen Method
mcvol	125.900	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
tb	603.46	K	Joback Method
tc	778.18	K	Joback Method
tf	388.83	K	Joback Method
vc	0.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.12	J/mol×K	603.46	Joback Method
cpg	302.87	J/mol×K	632.58	Joback Method
cpg	309.27	J/mol×K	661.70	Joback Method
cpg	315.35	J/mol×K	690.82	Joback Method
cpg	321.11	J/mol×K	719.94	Joback Method
cpg	326.57	J/mol×K	749.06	Joback Method
cpg	331.72	J/mol×K	778.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C719608&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

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