3-Pentafluorophenylpropionic acid

Inchi: InChI=1S/C9H5F5O2/c10-5-3(1-2-4(15)16)6(11)8(13)9(14)7(5)12/h1-2H2,(H,15,16)
InchiKey: KBAMYOFXGBJADC-UHFFFAOYSA-N
Formula: C9H5F5O2
SMILES: O=C(O)CCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 240.13
CAS: 2002-94-0

Physical Properties

Property code	Value	Unit	Source
gf	-1150.63	kJ/mol	Joback Method
hf	-1295.27	kJ/mol	Joback Method
hfus	32.25	kJ/mol	Joback Method
hvap	60.55	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	2.399		Crippen Method
mcvol	130.200	ml/mol	McGowan Method
pc	2781.78	kPa	Joback Method
tb	599.30	K	Joback Method
tc	768.13	K	Joback Method
tf	393.91	K	Joback Method
vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.22	J/mol×K	599.30	Joback Method
cpg	324.61	J/mol×K	627.44	Joback Method
cpg	331.69	J/mol×K	655.58	Joback Method
cpg	338.43	J/mol×K	683.71	Joback Method
cpg	344.86	J/mol×K	711.85	Joback Method
cpg	350.96	J/mol×K	739.99	Joback Method
cpg	356.75	J/mol×K	768.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2002940&Units=SI&Mask=3FFF
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