2-(Pentafluorophenyl)acetamide

Inchi: InChI=1S/C8H4F5NO/c9-4-2(1-3(14)15)5(10)7(12)8(13)6(4)11/h1H2,(H2,14,15)
InchiKey: DGTVZQUNYUHWBK-UHFFFAOYSA-N
Formula: C8H4F5NO
SMILES: NC(=O)Cc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 225.12
CAS: 653-20-3

Physical Properties

Property code	Value	Unit	Source
gf	-955.78	kJ/mol	Joback Method
hf	-1088.61	kJ/mol	Joback Method
hfus	30.77	kJ/mol	Joback Method
hvap	52.29	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	1.410		Crippen Method
mcvol	120.220	ml/mol	McGowan Method
pc	2969.80	kPa	Joback Method
tb	556.77	K	Joback Method
tc	743.15	K	Joback Method
tf	405.08	K	Joback Method
vc	0.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.14	J/mol×K	556.77	Joback Method
cpg	288.90	J/mol×K	587.83	Joback Method
cpg	296.31	J/mol×K	618.90	Joback Method
cpg	303.35	J/mol×K	649.96	Joback Method
cpg	310.03	J/mol×K	681.02	Joback Method
cpg	316.36	J/mol×K	712.08	Joback Method
cpg	322.34	J/mol×K	743.15	Joback Method

Sources

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=C653203&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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