Hydrocinnamamide, 2,3,4,5,6-pentafluoro-

Inchi: InChI=1S/C9H6F5NO/c10-5-3(1-2-4(15)16)6(11)8(13)9(14)7(5)12/h1-2H2,(H2,15,16)
InchiKey: SQAOPJSPFRAAKB-UHFFFAOYSA-N
Formula: C9H6F5NO
SMILES: NC(=O)CCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 239.14
CAS: 1994-24-7

Physical Properties

Property code	Value	Unit	Source
gf	-947.36	kJ/mol	Joback Method
hf	-1109.25	kJ/mol	Joback Method
hfus	33.36	kJ/mol	Joback Method
hvap	54.52	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	1.800		Crippen Method
mcvol	134.310	ml/mol	McGowan Method
pc	2681.86	kPa	Joback Method
tb	579.65	K	Joback Method
tc	764.03	K	Joback Method
tf	416.35	K	Joback Method
vc	0.556	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.09	J/mol×K	579.65	Joback Method
cpg	333.83	J/mol×K	610.38	Joback Method
cpg	342.15	J/mol×K	641.11	Joback Method
cpg	350.06	J/mol×K	671.84	Joback Method
cpg	357.57	J/mol×K	702.57	Joback Method
cpg	364.68	J/mol×K	733.30	Joback Method
cpg	371.39	J/mol×K	764.03	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=C1994247&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