Benzamide, pentafluoro-N-ethyl-

Inchi: InChI=1S/C9H6F5NO/c1-2-15-9(16)3-4(10)6(12)8(14)7(13)5(3)11/h2H2,1H3,(H,15,16)
InchiKey: JCKMCRGUKBTZRJ-UHFFFAOYSA-N
Formula: C9H6F5NO
SMILES: CCNC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 239.14

Physical Properties

Property code	Value	Unit	Source
gf	-924.42	kJ/mol	Joback Method
hf	-1089.57	kJ/mol	Joback Method
hfus	33.26	kJ/mol	Joback Method
hvap	50.31	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	2.132		Crippen Method
mcvol	134.310	ml/mol	McGowan Method
pc	2563.69	kPa	Joback Method
rinpol	1340.00		NIST Webbook
rinpol	1340.00		NIST Webbook
tb	557.29	K	Joback Method
tc	734.37	K	Joback Method
tf	385.75	K	Joback Method
vc	0.562	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.05	J/mol×K	557.29	Joback Method
cpg	325.97	J/mol×K	586.80	Joback Method
cpg	334.50	J/mol×K	616.32	Joback Method
cpg	342.64	J/mol×K	645.83	Joback Method
cpg	350.38	J/mol×K	675.34	Joback Method
cpg	357.75	J/mol×K	704.86	Joback Method
cpg	364.73	J/mol×K	734.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407934&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume