Benzamide, pentafluoro-N-methyl-

Inchi: InChI=1S/C8H4F5NO/c1-14-8(15)2-3(9)5(11)7(13)6(12)4(2)10/h1H3,(H,14,15)
InchiKey: AQQNFZYJRSIRRV-UHFFFAOYSA-N
Formula: C8H4F5NO
SMILES: CNC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 225.12

Physical Properties

Property code	Value	Unit	Source
gf	-932.84	kJ/mol	Joback Method
hf	-1068.93	kJ/mol	Joback Method
hfus	30.67	kJ/mol	Joback Method
hvap	48.08	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	1.742		Crippen Method
mcvol	120.220	ml/mol	McGowan Method
pc	2832.35	kPa	Joback Method
rinpol	1302.00		NIST Webbook
rinpol	1302.00		NIST Webbook
tb	534.41	K	Joback Method
tc	713.10	K	Joback Method
tf	374.48	K	Joback Method
vc	0.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.72	J/mol×K	534.41	Joback Method
cpg	281.66	J/mol×K	564.19	Joback Method
cpg	289.26	J/mol×K	593.97	Joback Method
cpg	296.52	J/mol×K	623.76	Joback Method
cpg	303.43	J/mol×K	653.54	Joback Method
cpg	310.01	J/mol×K	683.32	Joback Method
cpg	316.25	J/mol×K	713.10	Joback Method

Sources

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=U407933&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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