Benzamide, N-(4-fluorophenyl)-2,3,4-trifluoro-

Inchi: InChI=1S/C13H7F4NO/c14-7-1-3-8(4-2-7)18-13(19)9-5-6-10(15)12(17)11(9)16/h1-6H,(H
InchiKey: VYIIAWWHTUDYBL-UHFFFAOYSA-N
Formula: C13H7F4NO
SMILES: O=C(Nc1ccc(F)cc1)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 269.19

Physical Properties

Property code	Value	Unit	Source
gf	-573.89	kJ/mol	Joback Method
hf	-728.02	kJ/mol	Joback Method
hfus	34.97	kJ/mol	Joback Method
hvap	61.65	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	3.495		Crippen Method
mcvol	165.140	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
rinpol	1761.00		NIST Webbook
tb	671.24	K	Joback Method
tc	881.70	K	Joback Method
tf	444.14	K	Joback Method
vc	0.660	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.54	J/mol×K	671.24	Joback Method
cpg	429.70	J/mol×K	706.32	Joback Method
cpg	440.06	J/mol×K	741.39	Joback Method
cpg	449.66	J/mol×K	776.47	Joback Method
cpg	458.53	J/mol×K	811.55	Joback Method
cpg	466.70	J/mol×K	846.63	Joback Method
cpg	474.20	J/mol×K	881.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307174&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

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