Benzamide, N-(2-fluorophenyl)-2,6-difluoro-

Inchi: InChI=1S/C13H8F3NO/c14-8-4-1-2-7-11(8)17-13(18)12-9(15)5-3-6-10(12)16/h1-7H,(H,1
InchiKey: RFHHKXIJMGILJC-UHFFFAOYSA-N
Formula: C13H8F3NO
SMILES: O=C(Nc1ccccc1F)c1c(F)cccc1F
Mol. weight [g/mol]: 251.20

Physical Properties

Property code	Value	Unit	Source
gf	-369.45	kJ/mol	Joback Method
hf	-520.44	kJ/mol	Joback Method
hfus	32.28	kJ/mol	Joback Method
hvap	61.80	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	3.356		Crippen Method
mcvol	163.370	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
rinpol	1739.00		NIST Webbook
tb	666.99	K	Joback Method
tc	885.90	K	Joback Method
tf	431.03	K	Joback Method
vc	0.642	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.76	J/mol×K	666.99	Joback Method
cpg	423.65	J/mol×K	703.47	Joback Method
cpg	434.65	J/mol×K	739.96	Joback Method
cpg	444.80	J/mol×K	776.44	Joback Method
cpg	454.15	J/mol×K	812.93	Joback Method
cpg	462.74	J/mol×K	849.41	Joback Method
cpg	470.60	J/mol×K	885.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308663&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