Benzamide, N-(4-fluorophenyl)-2-fluoro-

Inchi: InChI=1S/C13H9F2NO/c14-9-5-7-10(8-6-9)16-13(17)11-3-1-2-4-12(11)15/h1-8H,(H,16,1
InchiKey: YSRSFSHRXSKXNN-UHFFFAOYSA-N
Formula: C13H9F2NO
SMILES: O=C(Nc1ccc(F)cc1)c1ccccc1F
Mol. weight [g/mol]: 233.21

Physical Properties

Property code	Value	Unit	Source
gf	-165.01	kJ/mol	Joback Method
hf	-312.86	kJ/mol	Joback Method
hfus	29.59	kJ/mol	Joback Method
hvap	61.96	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.217		Crippen Method
mcvol	161.600	ml/mol	McGowan Method
pc	2928.17	kPa	Joback Method
rinpol	1817.00		NIST Webbook
rinpol	1817.00		NIST Webbook
tb	662.74	K	Joback Method
tc	890.89	K	Joback Method
tf	417.92	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.92	J/mol×K	662.74	Joback Method
cpg	417.60	J/mol×K	700.77	Joback Method
cpg	429.30	J/mol×K	738.79	Joback Method
cpg	440.05	J/mol×K	776.82	Joback Method
cpg	449.92	J/mol×K	814.84	Joback Method
cpg	458.94	J/mol×K	852.87	Joback Method
cpg	467.18	J/mol×K	890.89	Joback Method

Sources

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=U307079&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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