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

Inchi: InChI=1S/C15H14FNO/c1-2-11-7-9-12(10-8-11)15(18)17-14-6-4-3-5-13(14)16/h3-10H,2H
InchiKey: DWXWTDWAJVHBQZ-UHFFFAOYSA-N
Formula: C15H14FNO
SMILES: CCc1ccc(C(=O)Nc2ccccc2F)cc1
Mol. weight [g/mol]: 243.28

Physical Properties

Property code	Value	Unit	Source
gf	46.64	kJ/mol	Joback Method
hf	-158.03	kJ/mol	Joback Method
hfus	31.69	kJ/mol	Joback Method
hvap	67.22	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	3.640		Crippen Method
mcvol	188.010	ml/mol	McGowan Method
pc	2512.55	kPa	Joback Method
rinpol	2067.00		NIST Webbook
rinpol	2067.00		NIST Webbook
tb	709.23	K	Joback Method
tc	939.06	K	Joback Method
tf	439.87	K	Joback Method
vc	0.719	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.80	J/mol×K	709.23	Joback Method
cpg	513.14	J/mol×K	747.54	Joback Method
cpg	526.39	J/mol×K	785.84	Joback Method
cpg	538.60	J/mol×K	824.15	Joback Method
cpg	549.84	J/mol×K	862.45	Joback Method
cpg	560.15	J/mol×K	900.76	Joback Method
cpg	569.61	J/mol×K	939.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308542&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

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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