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

Inchi: InChI=1S/C17H18FNO/c1-2-3-6-13-9-11-14(12-10-13)17(20)19-16-8-5-4-7-15(16)18/h4-5
InchiKey: WUFHGRSGAKGLSO-UHFFFAOYSA-N
Formula: C17H18FNO
SMILES: CCCCc1ccc(C(=O)Nc2ccccc2F)cc1
Mol. weight [g/mol]: 271.33

Physical Properties

Property code	Value	Unit	Source
gf	63.48	kJ/mol	Joback Method
hf	-199.31	kJ/mol	Joback Method
hfus	36.87	kJ/mol	Joback Method
hvap	71.68	kJ/mol	Joback Method
log10ws	-5.42		Crippen Method
logp	4.421		Crippen Method
mcvol	216.190	ml/mol	McGowan Method
pc	2090.75	kPa	Joback Method
rinpol	2277.00		NIST Webbook
rinpol	2277.00		NIST Webbook
tb	754.99	K	Joback Method
tc	977.23	K	Joback Method
tf	462.41	K	Joback Method
vc	0.831	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	605.66	J/mol×K	754.99	Joback Method
cpg	620.67	J/mol×K	792.03	Joback Method
cpg	634.58	J/mol×K	829.07	Joback Method
cpg	647.45	J/mol×K	866.11	Joback Method
cpg	659.34	J/mol×K	903.15	Joback Method
cpg	670.30	J/mol×K	940.19	Joback Method
cpg	680.41	J/mol×K	977.23	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=U308565&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