Benzamide, N-ethyl-N-(3-methylphenyl)-2-fluoro-

Inchi: InChI=1S/C16H16FNO/c1-3-18(13-8-6-7-12(2)11-13)16(19)14-9-4-5-10-15(14)17/h4-11H

InchiKey: GHVWFBDKKHYOBV-UHFFFAOYSA-N

Formula: C16H16FNO

SMILES: CCN(C(=O)c1ccccc1F)c1cccc(C)c1

Mol. weight [g/mol]: 257.30

Physical Properties

Property code	Value	Unit	Source
gf	76.45	kJ/mol	Joback Method
hf	-164.61	kJ/mol	Joback Method
hfus	32.20	kJ/mol	Joback Method
hvap	65.06	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	3.801		Crippen Method
mcvol	202.100	ml/mol	McGowan Method
pc	2254.67	kPa	Joback Method
rinpol	1828.00		NIST Webbook
rinpol	1828.00		NIST Webbook
tb	694.38	K	Joback Method
tc	918.50	K	Joback Method
tf	430.95	K	Joback Method
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.54	J/mol×K	694.38	Joback Method
cpg	553.21	J/mol×K	731.73	Joback Method
cpg	567.72	J/mol×K	769.09	Joback Method
cpg	581.13	J/mol×K	806.44	Joback Method
cpg	593.53	J/mol×K	843.79	Joback Method
cpg	604.97	J/mol×K	881.15	Joback Method
cpg	615.51	J/mol×K	918.50	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=U308093&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