Benzamide, N-ethyl-N-(3-methylphenyl)-2,6-difluoro-

Inchi: InChI=1S/C16H15F2NO/c1-3-19(12-7-4-6-11(2)10-12)16(20)15-13(17)8-5-9-14(15)18/h4

InchiKey: MJFSVBZICOYLPW-UHFFFAOYSA-N

Formula: C16H15F2NO

SMILES: CCN(C(=O)c1c(F)cccc1F)c1cccc(C)c1

Mol. weight [g/mol]: 275.29

Physical Properties

Property code	Value	Unit	Source
gf	-127.99	kJ/mol	Joback Method
hf	-372.19	kJ/mol	Joback Method
hfus	34.89	kJ/mol	Joback Method
hvap	64.90	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	3.940		Crippen Method
mcvol	203.870	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
rinpol	1750.00		NIST Webbook
rinpol	1750.00		NIST Webbook
tb	698.63	K	Joback Method
tc	914.22	K	Joback Method
tf	444.06	K	Joback Method
vc	0.775	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.59	J/mol×K	698.63	Joback Method
cpg	559.37	J/mol×K	734.56	Joback Method
cpg	573.11	J/mol×K	770.49	Joback Method
cpg	585.86	J/mol×K	806.42	Joback Method
cpg	597.67	J/mol×K	842.36	Joback Method
cpg	608.61	J/mol×K	878.29	Joback Method
cpg	618.71	J/mol×K	914.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308665&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