Benzamide, N-ethyl-N-(3-methylphenyl)-2,3,4-trifluoro-

Inchi: InChI=1S/C16H14F3NO/c1-3-20(11-6-4-5-10(2)9-11)16(21)12-7-8-13(17)15(19)14(12)18

InchiKey: FKOGDUWKXPRXQB-UHFFFAOYSA-N

Formula: C16H14F3NO

SMILES: CCN(C(=O)c1ccc(F)c(F)c1F)c1cccc(C)c1

Mol. weight [g/mol]: 293.28

Physical Properties

Property code	Value	Unit	Source
gf	-332.43	kJ/mol	Joback Method
hf	-579.77	kJ/mol	Joback Method
hfus	37.58	kJ/mol	Joback Method
hvap	64.75	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.079		Crippen Method
mcvol	205.640	ml/mol	McGowan Method
pc	2018.13	kPa	Joback Method
rinpol	1763.00		NIST Webbook
rinpol	1763.00		NIST Webbook
tb	702.88	K	Joback Method
tc	910.73	K	Joback Method
tf	457.17	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	551.57	J/mol×K	702.88	Joback Method
cpg	565.56	J/mol×K	737.52	Joback Method
cpg	578.59	J/mol×K	772.16	Joback Method
cpg	590.72	J/mol×K	806.80	Joback Method
cpg	602.00	J/mol×K	841.45	Joback Method
cpg	612.45	J/mol×K	876.09	Joback Method
cpg	622.13	J/mol×K	910.73	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=U308419&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