Benzamide, N-ethyl-N-(3-methylphenyl)-3-trifluoromethyl-

Inchi: InChI=1S/C17H16F3NO/c1-3-21(15-9-4-6-12(2)10-15)16(22)13-7-5-8-14(11-13)17(18,19

InchiKey: PMWJHGOYRFZHOP-UHFFFAOYSA-N

Formula: C17H16F3NO

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

Mol. weight [g/mol]: 307.31

Physical Properties

Property code	Value	Unit	Source
gf	-301.91	kJ/mol	Joback Method
hf	-586.22	kJ/mol	Joback Method
hfus	33.54	kJ/mol	Joback Method
hvap	64.35	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.681		Crippen Method
mcvol	219.730	ml/mol	McGowan Method
pc	1935.54	kPa	Joback Method
rinpol	1770.00		NIST Webbook
tb	712.57	K	Joback Method
tc	926.12	K	Joback Method
tf	445.82	K	Joback Method
vc	0.839	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	609.14	J/mol×K	712.57	Joback Method
cpg	624.19	J/mol×K	748.16	Joback Method
cpg	638.10	J/mol×K	783.75	Joback Method
cpg	650.96	J/mol×K	819.35	Joback Method
cpg	662.84	J/mol×K	854.94	Joback Method
cpg	673.84	J/mol×K	890.53	Joback Method
cpg	684.03	J/mol×K	926.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308224&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