Benzamide, 4-(trifluoromethyl)-N-butyl-N-methyl-

Inchi: InChI=1S/C13H16F3NO/c1-3-4-9-17(2)12(18)10-5-7-11(8-6-10)13(14,15)16/h5-8H,3-4,9
InchiKey: FPFNPECANBTGOU-UHFFFAOYSA-N
Formula: C13H16F3NO
SMILES: CCCCN(C)C(=O)c1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]: 259.27

Physical Properties

Property code	Value	Unit	Source
gf	-438.37	kJ/mol	Joback Method
hf	-728.72	kJ/mol	Joback Method
hfus	29.52	kJ/mol	Joback Method
hvap	52.51	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.578		Crippen Method
mcvol	187.130	ml/mol	McGowan Method
pc	2056.76	kPa	Joback Method
rinpol	1760.00		NIST Webbook
rinpol	1760.00		NIST Webbook
tb	589.39	K	Joback Method
tc	776.96	K	Joback Method
tf	361.80	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.18	J/mol×K	589.39	Joback Method
cpg	496.18	J/mol×K	620.65	Joback Method
cpg	510.25	J/mol×K	651.91	Joback Method
cpg	523.44	J/mol×K	683.18	Joback Method
cpg	535.79	J/mol×K	714.44	Joback Method
cpg	547.35	J/mol×K	745.70	Joback Method
cpg	558.17	J/mol×K	776.96	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415693&Units=SI

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