Benzamide, 3-trifluoromethyl-N,N-diethyl-

Inchi: InChI=1S/C12H14F3NO/c1-3-16(4-2)11(17)9-6-5-7-10(8-9)12(13,14)15/h5-8H,3-4H2,1-2
InchiKey: MSFWJWHVBDTGRO-UHFFFAOYSA-N
Formula: C12H14F3NO
SMILES: CCN(CC)C(=O)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 245.24

Physical Properties

Property code	Value	Unit	Source
gf	-446.79	kJ/mol	Joback Method
hf	-708.08	kJ/mol	Joback Method
hfus	26.93	kJ/mol	Joback Method
hvap	50.29	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.187		Crippen Method
mcvol	173.040	ml/mol	McGowan Method
pc	2248.26	kPa	Joback Method
rinpol	1625.00		NIST Webbook
rinpol	1625.00		NIST Webbook
tb	566.51	K	Joback Method
tc	756.25	K	Joback Method
tf	350.53	K	Joback Method
vc	0.666	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.98	J/mol×K	566.51	Joback Method
cpg	446.48	J/mol×K	598.13	Joback Method
cpg	460.06	J/mol×K	629.76	Joback Method
cpg	472.77	J/mol×K	661.38	Joback Method
cpg	484.65	J/mol×K	693.00	Joback Method
cpg	495.75	J/mol×K	724.63	Joback Method
cpg	506.11	J/mol×K	756.25	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=U415567&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