Benzamide, 3-trifluoromethyl-N-ethyl-N-methyl-

Inchi: InChI=1S/C11H12F3NO/c1-3-15(2)10(16)8-5-4-6-9(7-8)11(12,13)14/h4-7H,3H2,1-2H3

InchiKey: HCYJYRBBNVVAMZ-UHFFFAOYSA-N

Formula: C11H12F3NO

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

Mol. weight [g/mol]: 231.21

Physical Properties

Property code	Value	Unit	Source
gf	-455.21	kJ/mol	Joback Method
hf	-687.44	kJ/mol	Joback Method
hfus	24.34	kJ/mol	Joback Method
hvap	48.06	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	2.797		Crippen Method
mcvol	158.950	ml/mol	McGowan Method
pc	2467.81	kPa	Joback Method
rinpol	1588.00		NIST Webbook
rinpol	1588.00		NIST Webbook
tb	543.63	K	Joback Method
tc	735.72	K	Joback Method
tf	339.26	K	Joback Method
vc	0.611	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.31	J/mol×K	543.63	Joback Method
cpg	398.24	J/mol×K	575.64	Joback Method
cpg	411.26	J/mol×K	607.66	Joback Method
cpg	423.42	J/mol×K	639.67	Joback Method
cpg	434.76	J/mol×K	671.69	Joback Method
cpg	445.34	J/mol×K	703.70	Joback Method
cpg	455.19	J/mol×K	735.72	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=U415566&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

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