Benzamide, 3-trifluoromethyl-N-ethyl-N-3-methylbutyl-

Inchi: InChI=1S/C15H20F3NO/c1-4-19(9-8-11(2)3)14(20)12-6-5-7-13(10-12)15(16,17)18/h5-7,1

InchiKey: GXXVUAJGXLPJCC-UHFFFAOYSA-N

Formula: C15H20F3NO

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

Mol. weight [g/mol]: 287.32

Physical Properties

Property code	Value	Unit	Source
gf	-423.97	kJ/mol	Joback Method
hf	-775.28	kJ/mol	Joback Method
hfus	31.18	kJ/mol	Joback Method
hvap	56.58	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	4.214		Crippen Method
mcvol	215.310	ml/mol	McGowan Method
pc	1752.14	kPa	Joback Method
rinpol	1882.00		NIST Webbook
rinpol	1882.00		NIST Webbook
tb	634.71	K	Joback Method
tc	821.77	K	Joback Method
tf	369.34	K	Joback Method
vc	0.829	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	584.31	J/mol×K	634.71	Joback Method
cpg	600.43	J/mol×K	665.89	Joback Method
cpg	615.56	J/mol×K	697.06	Joback Method
cpg	629.76	J/mol×K	728.24	Joback Method
cpg	643.08	J/mol×K	759.42	Joback Method
cpg	655.58	J/mol×K	790.59	Joback Method
cpg	667.29	J/mol×K	821.77	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=U415571&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