Benzamide, 3-trifluoromethyl-N-ethyl-N-isobutyl-

Inchi: InChI=1S/C14H18F3NO/c1-4-18(9-10(2)3)13(19)11-6-5-7-12(8-11)14(15,16)17/h5-8,10H

InchiKey: PDMJCVJBXYWJDH-UHFFFAOYSA-N

Formula: C14H18F3NO

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

Mol. weight [g/mol]: 273.29

Physical Properties

Property code	Value	Unit	Source
gf	-432.39	kJ/mol	Joback Method
hf	-754.64	kJ/mol	Joback Method
hfus	28.59	kJ/mol	Joback Method
hvap	54.35	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.824		Crippen Method
mcvol	201.220	ml/mol	McGowan Method
pc	1901.92	kPa	Joback Method
rinpol	1728.00		NIST Webbook
rinpol	1728.00		NIST Webbook
tb	611.83	K	Joback Method
tc	800.78	K	Joback Method
tf	358.07	K	Joback Method
vc	0.772	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	532.25	J/mol×K	611.83	Joback Method
cpg	548.00	J/mol×K	643.32	Joback Method
cpg	562.78	J/mol×K	674.81	Joback Method
cpg	576.62	J/mol×K	706.30	Joback Method
cpg	589.59	J/mol×K	737.80	Joback Method
cpg	601.73	J/mol×K	769.29	Joback Method
cpg	613.09	J/mol×K	800.78	Joback Method

Sources

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=U415569&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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