Benzamide, 2,3,4-trifluoro-N-butyl-N-ethyl-

Inchi: InChI=1S/C13H16F3NO/c1-3-5-8-17(4-2)13(18)9-6-7-10(14)12(16)11(9)15/h6-7H,3-5,8H
InchiKey: FHVPXZHQYVVOJH-UHFFFAOYSA-N
Formula: C13H16F3NO
SMILES: CCCCN(CC)C(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 259.27

Physical Properties

Property code	Value	Unit	Source
gf	-460.47	kJ/mol	Joback Method
hf	-742.91	kJ/mol	Joback Method
hfus	36.16	kJ/mol	Joback Method
hvap	55.13	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	3.366		Crippen Method
mcvol	187.130	ml/mol	McGowan Method
pc	1968.30	kPa	Joback Method
rinpol	1789.00		NIST Webbook
rinpol	1789.00		NIST Webbook
tb	602.58	K	Joback Method
tc	782.81	K	Joback Method
tf	384.42	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	477.63	J/mol×K	602.58	Joback Method
cpg	491.49	J/mol×K	632.62	Joback Method
cpg	504.64	J/mol×K	662.66	Joback Method
cpg	517.10	J/mol×K	692.70	Joback Method
cpg	528.91	J/mol×K	722.74	Joback Method
cpg	540.07	J/mol×K	752.78	Joback Method
cpg	550.62	J/mol×K	782.81	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=U415677&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