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

Inchi: InChI=1S/C11H12F3NO/c1-2-3-6-15-11(16)7-4-5-8(12)10(14)9(7)13/h4-5H,2-3,6H2,1H3,
InchiKey: ONRDKYORXBEDAZ-UHFFFAOYSA-N
Formula: C11H12F3NO
SMILES: CCCCNC(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 231.21

Physical Properties

Property code	Value	Unit	Source
gf	-498.70	kJ/mol	Joback Method
hf	-715.69	kJ/mol	Joback Method
hfus	33.06	kJ/mol	Joback Method
hvap	55.07	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	2.634		Crippen Method
mcvol	158.950	ml/mol	McGowan Method
pc	2386.52	kPa	Joback Method
rinpol	1524.00		NIST Webbook
rinpol	1524.00		NIST Webbook
tb	594.55	K	Joback Method
tc	781.79	K	Joback Method
tf	382.07	K	Joback Method
vc	0.638	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.19	J/mol×K	594.55	Joback Method
cpg	406.17	J/mol×K	625.76	Joback Method
cpg	417.53	J/mol×K	656.96	Joback Method
cpg	428.29	J/mol×K	688.17	Joback Method
cpg	438.46	J/mol×K	719.38	Joback Method
cpg	448.06	J/mol×K	750.59	Joback Method
cpg	457.11	J/mol×K	781.79	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=U407260&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