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

Inchi: InChI=1S/C11H12F3NO/c1-6(2)5-15-11(16)7-3-4-8(12)10(14)9(7)13/h3-4,6H,5H2,1-2H3,
InchiKey: NSJSIADGPWENFX-UHFFFAOYSA-N
Formula: C11H12F3NO
SMILES: CC(C)CNC(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 231.21

Physical Properties

Property code	Value	Unit	Source
gf	-501.14	kJ/mol	Joback Method
hf	-720.97	kJ/mol	Joback Method
hfus	29.54	kJ/mol	Joback Method
hvap	54.69	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	2.490		Crippen Method
mcvol	158.950	ml/mol	McGowan Method
pc	2405.28	kPa	Joback Method
rinpol	1473.00		NIST Webbook
rinpol	1473.00		NIST Webbook
tb	594.11	K	Joback Method
tc	784.85	K	Joback Method
tf	367.07	K	Joback Method
vc	0.632	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.62	J/mol×K	594.11	Joback Method
cpg	406.87	J/mol×K	625.90	Joback Method
cpg	418.47	J/mol×K	657.69	Joback Method
cpg	429.44	J/mol×K	689.48	Joback Method
cpg	439.79	J/mol×K	721.27	Joback Method
cpg	449.55	J/mol×K	753.06	Joback Method
cpg	458.72	J/mol×K	784.85	Joback Method

Sources

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=U407259&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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