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

Inchi: InChI=1S/C12H14F3NO/c1-3-4-7-16(2)12(17)8-5-6-9(13)11(15)10(8)14/h5-6H,3-4,7H2,1
InchiKey: YSLZNDNPJPBTBX-UHFFFAOYSA-N
Formula: C12H14F3NO
SMILES: CCCCN(C)C(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 245.24

Physical Properties

Property code	Value	Unit	Source
gf	-468.89	kJ/mol	Joback Method
hf	-722.27	kJ/mol	Joback Method
hfus	33.57	kJ/mol	Joback Method
hvap	52.91	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	2.976		Crippen Method
mcvol	173.040	ml/mol	McGowan Method
pc	2147.32	kPa	Joback Method
rinpol	1736.00		NIST Webbook
rinpol	1736.00		NIST Webbook
tb	579.70	K	Joback Method
tc	761.56	K	Joback Method
tf	373.15	K	Joback Method
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.38	J/mol×K	579.70	Joback Method
cpg	441.62	J/mol×K	610.01	Joback Method
cpg	454.18	J/mol×K	640.32	Joback Method
cpg	466.09	J/mol×K	670.63	Joback Method
cpg	477.36	J/mol×K	700.94	Joback Method
cpg	488.01	J/mol×K	731.25	Joback Method
cpg	498.07	J/mol×K	761.56	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=U415676&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