Benzamide, 2,3,4-trifluoro-N-(3-methylbutyl)-

Inchi: InChI=1S/C12H14F3NO/c1-7(2)5-6-16-12(17)8-3-4-9(13)11(15)10(8)14/h3-4,7H,5-6H2,1
InchiKey: AKYCBSIFPZAZAY-UHFFFAOYSA-N
Formula: C12H14F3NO
SMILES: CC(C)CCNC(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 245.24

Physical Properties

Property code	Value	Unit	Source
gf	-492.72	kJ/mol	Joback Method
hf	-741.61	kJ/mol	Joback Method
hfus	32.12	kJ/mol	Joback Method
hvap	56.91	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	2.880		Crippen Method
mcvol	173.040	ml/mol	McGowan Method
pc	2193.84	kPa	Joback Method
rinpol	1585.00		NIST Webbook
rinpol	1585.00		NIST Webbook
tb	616.99	K	Joback Method
tc	805.61	K	Joback Method
tf	378.34	K	Joback Method
vc	0.689	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.29	J/mol×K	616.99	Joback Method
cpg	456.22	J/mol×K	648.43	Joback Method
cpg	468.46	J/mol×K	679.86	Joback Method
cpg	480.03	J/mol×K	711.30	Joback Method
cpg	490.96	J/mol×K	742.74	Joback Method
cpg	501.26	J/mol×K	774.17	Joback Method
cpg	510.95	J/mol×K	805.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407261&Units=SI
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

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