Benzamide, 2,4,5-trifluoro-3-methoxy-N-(3-methylbutyl)-

Inchi: InChI=1S/C13H16F3NO2/c1-7(2)4-5-17-13(18)8-6-9(14)11(16)12(19-3)10(8)15/h6-7H,4-

InchiKey: CQISMWWHTPJOEC-UHFFFAOYSA-N

Formula: C13H16F3NO2

SMILES: COc1c(F)c(F)cc(C(=O)NCCC(C)C)c1F

Mol. weight [g/mol]: 275.27

Physical Properties

Property code	Value	Unit	Source
gf	-598.93	kJ/mol	Joback Method
hf	-905.94	kJ/mol	Joback Method
hfus	35.51	kJ/mol	Joback Method
hvap	62.21	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	2.888		Crippen Method
mcvol	193.000	ml/mol	McGowan Method
pc	1952.68	kPa	Joback Method
rinpol	1786.00		NIST Webbook
rinpol	1786.00		NIST Webbook
tb	667.27	K	Joback Method
tc	854.16	K	Joback Method
tf	424.36	K	Joback Method
vc	0.762	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.96	J/mol×K	667.27	Joback Method
cpg	532.14	J/mol×K	698.42	Joback Method
cpg	544.64	J/mol×K	729.57	Joback Method
cpg	556.46	J/mol×K	760.72	Joback Method
cpg	567.62	J/mol×K	791.86	Joback Method
cpg	578.12	J/mol×K	823.01	Joback Method
cpg	587.96	J/mol×K	854.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407639&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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