Benzamide, 2,4,5-trifluoro-3-methoxy-N-methyl-

Inchi: InChI=1S/C9H8F3NO2/c1-13-9(14)4-3-5(10)7(12)8(15-2)6(4)11/h3H,1-2H3,(H,13,14)
InchiKey: UDMIWHRSILLBES-UHFFFAOYSA-N
Formula: C9H8F3NO2
SMILES: CNC(=O)c1cc(F)c(F)c(OC)c1F
Mol. weight [g/mol]: 219.16

Physical Properties

Property code	Value	Unit	Source
gf	-630.17	kJ/mol	Joback Method
hf	-818.10	kJ/mol	Joback Method
hfus	28.68	kJ/mol	Joback Method
hvap	53.69	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	1.472		Crippen Method
mcvol	136.640	ml/mol	McGowan Method
pc	2808.38	kPa	Joback Method
rinpol	1493.00		NIST Webbook
rinpol	1493.00		NIST Webbook
tb	576.19	K	Joback Method
tc	767.48	K	Joback Method
tf	394.28	K	Joback Method
vc	0.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.73	J/mol×K	576.19	Joback Method
cpg	333.73	J/mol×K	608.07	Joback Method
cpg	343.27	J/mol×K	639.95	Joback Method
cpg	352.36	J/mol×K	671.83	Joback Method
cpg	360.98	J/mol×K	703.72	Joback Method
cpg	369.14	J/mol×K	735.60	Joback Method
cpg	376.84	J/mol×K	767.48	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=U407634&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