Benzamide, 2,4,5-trifluoro-3-methoxy-N-(2,4,5-trifluoro-3-meth

Inchi: InChI=1S/C19H15F6NO4/c1-4-5-26(18(27)8-6-10(20)14(24)16(29-2)12(8)22)19(28)9-7-1

InchiKey: NWOHTWXVBRTQCO-UHFFFAOYSA-N

Formula: C19H15F6NO4

SMILES: CCCN(C(=O)c1cc(F)c(F)c(OC)c1F)C(=O)c1cc(F)c(F)c(OC)c1F

Mol. weight [g/mol]: 435.32

Physical Properties

Property code	Value	Unit	Source
gf	-1269.04	kJ/mol	Joback Method
hf	-1652.92	kJ/mol	Joback Method
hfus	57.01	kJ/mol	Joback Method
hvap	83.19	kJ/mol	Joback Method
log10ws	-6.65		Crippen Method
logp	4.231		Crippen Method
mcvol	266.530	ml/mol	McGowan Method
pc	1392.29	kPa	Joback Method
rinpol	2148.00		NIST Webbook
rinpol	2148.00		NIST Webbook
tb	887.96	K	Joback Method
tc	1090.44	K	Joback Method
tf	637.22	K	Joback Method
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	800.75	J/mol×K	887.96	Joback Method
cpg	811.88	J/mol×K	921.71	Joback Method
cpg	821.96	J/mol×K	955.45	Joback Method
cpg	831.00	J/mol×K	989.20	Joback Method
cpg	838.99	J/mol×K	1022.94	Joback Method
cpg	845.95	J/mol×K	1056.69	Joback Method
cpg	851.87	J/mol×K	1090.44	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=U407655&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