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

Inchi: InChI=1S/C21H19F6NO4/c1-4-5-6-7-28(20(29)10-8-12(22)16(26)18(31-2)14(10)24)21(30

InchiKey: BDKKETQIVBHZIQ-UHFFFAOYSA-N

Formula: C21H19F6NO4

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

Mol. weight [g/mol]: 463.37

Physical Properties

Property code	Value	Unit	Source
gf	-1252.20	kJ/mol	Joback Method
hf	-1694.20	kJ/mol	Joback Method
hfus	62.19	kJ/mol	Joback Method
hvap	87.64	kJ/mol	Joback Method
log10ws	-7.49		Crippen Method
logp	5.011		Crippen Method
mcvol	294.710	ml/mol	McGowan Method
pc	1212.36	kPa	Joback Method
rinpol	2323.00		NIST Webbook
rinpol	2323.00		NIST Webbook
tb	933.72	K	Joback Method
tc	1143.34	K	Joback Method
tf	659.76	K	Joback Method
vc	1.169	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	915.70	J/mol×K	933.72	Joback Method
cpg	927.39	J/mol×K	968.66	Joback Method
cpg	937.88	J/mol×K	1003.59	Joback Method
cpg	947.15	J/mol×K	1038.53	Joback Method
cpg	955.23	J/mol×K	1073.47	Joback Method
cpg	962.11	J/mol×K	1108.40	Joback Method
cpg	967.82	J/mol×K	1143.34	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=U407659&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