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

Inchi: InChI=1S/C25H27F6NO4/c1-4-5-6-7-8-9-10-11-32(24(33)14-12-16(26)20(30)22(35-2)18(

InchiKey: CIRKJBDSESIKAL-UHFFFAOYSA-N

Formula: C25H27F6NO4

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

Mol. weight [g/mol]: 519.48

Physical Properties

Property code	Value	Unit	Source
gf	-1218.52	kJ/mol	Joback Method
hf	-1776.76	kJ/mol	Joback Method
hfus	72.55	kJ/mol	Joback Method
hvap	96.55	kJ/mol	Joback Method
log10ws	-9.16		Crippen Method
logp	6.572		Crippen Method
mcvol	351.070	ml/mol	McGowan Method
pc	943.26	kPa	Joback Method
tb	1025.24	K	Joback Method
tc	1261.41	K	Joback Method
tf	704.84	K	Joback Method
vc	1.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1152.29	J/mol×K	1025.24	Joback Method
cpg	1165.01	J/mol×K	1064.60	Joback Method
cpg	1176.02	J/mol×K	1103.96	Joback Method
cpg	1185.34	J/mol×K	1143.32	Joback Method
cpg	1193.00	J/mol×K	1182.69	Joback Method
cpg	1199.04	J/mol×K	1222.05	Joback Method
cpg	1203.48	J/mol×K	1261.41	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=U407665&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume