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

Inchi: InChI=1S/C26H29F6NO4/c1-4-5-6-7-8-9-10-11-12-33(25(34)15-13-17(27)21(31)23(36-2)

InchiKey: RLTVQCDBEVOGCS-UHFFFAOYSA-N

Formula: C26H29F6NO4

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

Mol. weight [g/mol]: 533.50

Physical Properties

Property code	Value	Unit	Source
gf	-1210.10	kJ/mol	Joback Method
hf	-1797.40	kJ/mol	Joback Method
hfus	75.14	kJ/mol	Joback Method
hvap	98.77	kJ/mol	Joback Method
log10ws	-9.58		Crippen Method
logp	6.962		Crippen Method
mcvol	365.160	ml/mol	McGowan Method
pc	890.00	kPa	Joback Method
rinpol	2818.00		NIST Webbook
tb	1048.12	K	Joback Method
tc	1293.95	K	Joback Method
tf	716.11	K	Joback Method
vc	1.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1212.50	J/mol×K	1048.12	Joback Method
cpg	1225.46	J/mol×K	1089.09	Joback Method
cpg	1236.54	J/mol×K	1130.06	Joback Method
cpg	1245.75	J/mol×K	1171.03	Joback Method
cpg	1253.16	J/mol×K	1212.01	Joback Method
cpg	1258.79	J/mol×K	1252.98	Joback Method
cpg	1262.68	J/mol×K	1293.95	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=U407666&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