

Benzamide, 2,4,5-trifluoro-3-methoxy-N-(2,4,5-trifluoro-3-methoxyphenyl)

Inchi: InChI=1S/C24H25F6NO4/c1-4-5-6-7-8-9-10-31(23(32)13-11-15(25)19(29)21(34-2)17(13)-22)24

InchiKey: BZVPEGMJNZLINJ-UHFFFAOYSA-N

Formula: C₂₄H₂₅F₆NO₄

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

Mol. weight [g/mol]: 505.45

Physical Properties

Property code	Value	Unit	Source
gf	-1226.94	kJ/mol	Joback Method
hf	-1756.12	kJ/mol	Joback Method
hfus	69.96	kJ/mol	Joback Method
hvap	94.32	kJ/mol	Joback Method
log10ws	-8.74		Crippen Method
logp	6.182		Crippen Method
mcvol	336.980	ml/mol	McGowan Method
pc	1001.44	kPa	Joback Method
rinpol	2616.00		NIST Webbook
rinpol	2616.00		NIST Webbook
tb	1002.36	K	Joback Method
tc	1230.17	K	Joback Method
tf	693.57	K	Joback Method
vc	1.337	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1092.45	J/molxK	1002.36	Joback Method
cpg	1104.93	J/molxK	1040.33	Joback Method
cpg	1115.84	J/molxK	1078.30	Joback Method
cpg	1125.21	J/molxK	1116.26	Joback Method
cpg	1133.06	J/molxK	1154.23	Joback Method
cpg	1139.42	J/molxK	1192.20	Joback Method
cpg	1144.30	J/molxK	1230.17	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U407664&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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