

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

Inchi: InChI=1S/C32H41F6NO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-39(31(40)21-19-20)22-23-24-25-26-27-28-29-30

InchiKey: CNTKOPKQZRUFCE-UHFFFAOYSA-N

Formula: C32H41F6NO4

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

Mol. weight [g/mol]: 617.66

Physical Properties

Property code	Value	Unit	Source
gf	-1159.58	kJ/mol	Joback Method
hf	-1921.24	kJ/mol	Joback Method
hfus	90.68	kJ/mol	Joback Method
hvap	112.13	kJ/mol	Joback Method
log10ws	-12.09		Crippen Method
logp	9.302		Crippen Method
mvol	449.700	ml/mol	McGowan Method
pc	648.12	kPa	Joback Method
rinpol	3432.00		NIST Webbook
tb	1185.40	K	Joback Method
tc	1522.73	K	Joback Method
tf	783.73	K	Joback Method
vc	1.786	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1579.06	J/molxK	1185.40	Joback Method
cpg	1593.15	J/molxK	1241.62	Joback Method
cpg	1603.57	J/molxK	1297.84	Joback Method
cpg	1610.50	J/molxK	1354.07	Joback Method
cpg	1614.10	J/molxK	1410.29	Joback Method
cpg	1614.55	J/molxK	1466.51	Joback Method
cpg	1612.03	J/molxK	1522.73	Joback Method

Sources

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=U407670&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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

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