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

Inchi: InChI=1S/C21H19F6NO4/c1-9(2)5-6-28(20(29)10-7-12(22)16(26)18(31-3)14(10)24)21(30

InchiKey: DBJQYFCHYMXTLM-UHFFFAOYSA-N

Formula: C21H19F6NO4

SMILES: COc1c(F)c(F)cc(C(=O)N(CCC(C)C)C(=O)c2cc(F)c(F)c(OC)c2F)c1F

Mol. weight [g/mol]: 463.37

Physical Properties

Property code	Value	Unit	Source
gf	-1254.64	kJ/mol	Joback Method
hf	-1699.48	kJ/mol	Joback Method
hfus	58.67	kJ/mol	Joback Method
hvap	87.25	kJ/mol	Joback Method
log10ws	-7.24		Crippen Method
logp	4.867		Crippen Method
mcvol	294.710	ml/mol	McGowan Method
pc	1219.14	kPa	Joback Method
rinpol	2279.00		NIST Webbook
rinpol	2279.00		NIST Webbook
tb	933.28	K	Joback Method
tc	1143.12	K	Joback Method
tf	644.76	K	Joback Method
vc	1.163	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	916.19	J/mol×K	933.28	Joback Method
cpg	927.86	J/mol×K	968.25	Joback Method
cpg	938.30	J/mol×K	1003.23	Joback Method
cpg	947.52	J/mol×K	1038.20	Joback Method
cpg	955.53	J/mol×K	1073.18	Joback Method
cpg	962.34	J/mol×K	1108.15	Joback Method
cpg	967.94	J/mol×K	1143.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407658&Units=SI
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

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

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