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

Inchi: InChI=1S/C18H13F6NO4/c1-4-25(17(26)7-5-9(19)13(23)15(28-2)11(7)21)18(27)8-6-10(2

InchiKey: GQKLDGJJKVMIDH-UHFFFAOYSA-N

Formula: C18H13F6NO4

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

Mol. weight [g/mol]: 421.29

Physical Properties

Property code	Value	Unit	Source
gf	-1277.46	kJ/mol	Joback Method
hf	-1632.28	kJ/mol	Joback Method
hfus	54.42	kJ/mol	Joback Method
hvap	80.96	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	3.841		Crippen Method
mcvol	252.440	ml/mol	McGowan Method
pc	1497.67	kPa	Joback Method
rinpol	2070.00		NIST Webbook
rinpol	2070.00		NIST Webbook
tb	865.08	K	Joback Method
tc	1065.27	K	Joback Method
tf	625.95	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	744.34	J/mol×K	865.08	Joback Method
cpg	755.16	J/mol×K	898.45	Joback Method
cpg	765.00	J/mol×K	931.81	Joback Method
cpg	773.87	J/mol×K	965.18	Joback Method
cpg	781.76	J/mol×K	998.54	Joback Method
cpg	788.67	J/mol×K	1031.91	Joback Method
cpg	794.61	J/mol×K	1065.27	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=U407654&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