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

Inchi: InChI=1S/C20H17F6NO4/c1-8(2)7-27(19(28)9-5-11(21)15(25)17(30-3)13(9)23)20(29)10-

InchiKey: CCOOBSOUNGIMDX-UHFFFAOYSA-N

Formula: C20H17F6NO4

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

Mol. weight [g/mol]: 449.34

Physical Properties

Property code	Value	Unit	Source
gf	-1263.06	kJ/mol	Joback Method
hf	-1678.84	kJ/mol	Joback Method
hfus	56.08	kJ/mol	Joback Method
hvap	85.03	kJ/mol	Joback Method
log10ws	-6.83		Crippen Method
logp	4.477		Crippen Method
mcvol	280.620	ml/mol	McGowan Method
pc	1305.17	kPa	Joback Method
rinpol	2184.00		NIST Webbook
rinpol	2184.00		NIST Webbook
tb	910.40	K	Joback Method
tc	1116.59	K	Joback Method
tf	633.49	K	Joback Method
vc	1.107	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	858.42	J/mol×K	910.40	Joback Method
cpg	869.84	J/mol×K	944.77	Joback Method
cpg	880.12	J/mol×K	979.13	Joback Method
cpg	889.25	J/mol×K	1013.50	Joback Method
cpg	897.26	J/mol×K	1047.86	Joback Method
cpg	904.14	J/mol×K	1082.23	Joback Method
cpg	909.89	J/mol×K	1116.59	Joback Method

Sources

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=U407656&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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