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

Inchi: InChI=1S/C17H11F6NO4/c1-24(16(25)6-4-8(18)12(22)14(27-2)10(6)20)17(26)7-5-9(19)1

InchiKey: ZNIIGQJNXPNTLN-UHFFFAOYSA-N

Formula: C17H11F6NO4

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

Mol. weight [g/mol]: 407.26

Physical Properties

Property code	Value	Unit	Source
gf	-1285.88	kJ/mol	Joback Method
hf	-1611.64	kJ/mol	Joback Method
hfus	51.83	kJ/mol	Joback Method
hvap	78.74	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	3.451		Crippen Method
mcvol	238.350	ml/mol	McGowan Method
pc	1615.47	kPa	Joback Method
rinpol	2053.00		NIST Webbook
rinpol	2053.00		NIST Webbook
tb	842.20	K	Joback Method
tc	1040.89	K	Joback Method
tf	614.68	K	Joback Method
vc	0.946	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.74	J/mol×K	842.20	Joback Method
cpg	699.22	J/mol×K	875.32	Joback Method
cpg	708.79	J/mol×K	908.43	Joback Method
cpg	717.44	J/mol×K	941.55	Joback Method
cpg	725.19	J/mol×K	974.66	Joback Method
cpg	732.01	J/mol×K	1007.78	Joback Method
cpg	737.91	J/mol×K	1040.89	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=U407653&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