2,4,5-Trifluoro-3-methoxybenzamide, N-(2,5-dimethoxyphenyl)-

Inchi: InChI=1S/C16H14F3NO4/c1-22-8-4-5-12(23-2)11(6-8)20-16(21)9-7-10(17)14(19)15(24-3

InchiKey: XSEUYVZDQHAXDR-UHFFFAOYSA-N

Formula: C16H14F3NO4

SMILES: COc1ccc(OC)c(NC(=O)c2cc(F)c(F)c(OC)c2F)c1

Mol. weight [g/mol]: 341.28

Physical Properties

Property code	Value	Unit	Source
gf	-688.08	kJ/mol	Joback Method
hf	-1013.43	kJ/mol	Joback Method
hfus	42.45	kJ/mol	Joback Method
hvap	77.69	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	3.382		Crippen Method
mcvol	223.250	ml/mol	McGowan Method
pc	1903.58	kPa	Joback Method
rinpol	2506.00		NIST Webbook
rinpol	2506.00		NIST Webbook
tb	817.83	K	Joback Method
tc	1026.52	K	Joback Method
tf	569.09	K	Joback Method
vc	0.865	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	640.93	J/mol×K	817.83	Joback Method
cpg	652.90	J/mol×K	852.61	Joback Method
cpg	663.84	J/mol×K	887.39	Joback Method
cpg	673.75	J/mol×K	922.18	Joback Method
cpg	682.62	J/mol×K	956.96	Joback Method
cpg	690.42	J/mol×K	991.74	Joback Method
cpg	697.13	J/mol×K	1026.52	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=U358070&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