3-Fluoro-6-trifluoromethylbenzamide, N-(2,5-dimethoxyphenyl)-

Inchi: InChI=1S/C16H13F4NO3/c1-23-10-4-6-14(24-2)13(8-10)21-15(22)11-7-9(17)3-5-12(11)1

InchiKey: NFLZGGYUUHKNPO-UHFFFAOYSA-N

Formula: C16H13F4NO3

SMILES: COc1ccc(OC)c(NC(=O)c2cc(F)ccc2C(F)(F)F)c1

Mol. weight [g/mol]: 343.27

Physical Properties

Property code	Value	Unit	Source
gf	-755.79	kJ/mol	Joback Method
hf	-1063.13	kJ/mol	Joback Method
hfus	37.70	kJ/mol	Joback Method
hvap	71.85	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.114		Crippen Method
mcvol	219.150	ml/mol	McGowan Method
pc	1938.95	kPa	Joback Method
rinpol	2196.00		NIST Webbook
rinpol	2196.00		NIST Webbook
tb	781.49	K	Joback Method
tc	990.63	K	Joback Method
tf	524.83	K	Joback Method
vc	0.854	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.09	J/mol×K	781.49	Joback Method
cpg	639.29	J/mol×K	816.35	Joback Method
cpg	650.52	J/mol×K	851.20	Joback Method
cpg	660.81	J/mol×K	886.06	Joback Method
cpg	670.19	J/mol×K	920.91	Joback Method
cpg	678.68	J/mol×K	955.77	Joback Method
cpg	686.32	J/mol×K	990.63	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=U358083&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