2,5-Difluorobenzamide, N-(2,5-dimethoxyphenyl)-

Inchi: InChI=1S/C15H13F2NO3/c1-20-10-4-6-14(21-2)13(8-10)18-15(19)11-7-9(16)3-5-12(11)1

InchiKey: VUXAXYVABLGRSS-UHFFFAOYSA-N

Formula: C15H13F2NO3

SMILES: COc1ccc(OC)c(NC(=O)c2cc(F)ccc2F)c1

Mol. weight [g/mol]: 293.27

Physical Properties

Property code	Value	Unit	Source
gf	-377.43	kJ/mol	Joback Method
hf	-641.52	kJ/mol	Joback Method
hfus	36.37	kJ/mol	Joback Method
hvap	72.55	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	3.234		Crippen Method
mcvol	201.520	ml/mol	McGowan Method
pc	2258.96	kPa	Joback Method
rinpol	2323.00		NIST Webbook
rinpol	2323.00		NIST Webbook
tb	763.30	K	Joback Method
tc	980.61	K	Joback Method
tf	509.96	K	Joback Method
vc	0.772	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.63	J/mol×K	763.30	Joback Method
cpg	568.33	J/mol×K	799.52	Joback Method
cpg	580.05	J/mol×K	835.74	Joback Method
cpg	590.80	J/mol×K	871.96	Joback Method
cpg	600.57	J/mol×K	908.18	Joback Method
cpg	609.37	J/mol×K	944.39	Joback Method
cpg	617.22	J/mol×K	980.61	Joback Method

Sources

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=U358049&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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