Benzamide, N-(2,5-dimethoxyphenyl)-4-fluoro-

Inchi: InChI=1S/C15H14FNO3/c1-19-12-7-8-14(20-2)13(9-12)17-15(18)10-3-5-11(16)6-4-10/h3
InchiKey: VJEIFAFFAAIGLK-UHFFFAOYSA-N
Formula: C15H14FNO3
SMILES: COc1ccc(OC)c(NC(=O)c2ccc(F)cc2)c1
Mol. weight [g/mol]: 275.27

Physical Properties

Property code	Value	Unit	Source
gf	-172.99	kJ/mol	Joback Method
hf	-433.94	kJ/mol	Joback Method
hfus	33.67	kJ/mol	Joback Method
hvap	72.71	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.095		Crippen Method
mcvol	199.750	ml/mol	McGowan Method
pc	2393.53	kPa	Joback Method
rinpol	2267.00		NIST Webbook
tb	759.05	K	Joback Method
tc	984.05	K	Joback Method
tf	496.85	K	Joback Method
vc	0.754	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	549.15	J/mol×K	759.05	Joback Method
cpg	562.56	J/mol×K	796.55	Joback Method
cpg	574.89	J/mol×K	834.05	Joback Method
cpg	586.17	J/mol×K	871.55	Joback Method
cpg	596.41	J/mol×K	909.05	Joback Method
cpg	605.62	J/mol×K	946.55	Joback Method
cpg	613.82	J/mol×K	984.05	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=U307106&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