Benzamide, n-(2,5-dimethoxyphenyl)-2-fluoro-

Inchi: InChI=1S/C15H14FNO3/c1-19-10-7-8-14(20-2)13(9-10)17-15(18)11-5-3-4-6-12(11)16/h3
InchiKey: SWDJJOROGFXGIT-UHFFFAOYSA-N
Formula: C15H14FNO3
SMILES: COc1ccc(OC)c(NC(=O)c2ccccc2F)c1
Mol. weight [g/mol]: 275.28

Physical Properties

Property code	Value	Unit	Source
hf	-482.90	kJ/mol	Cheméo Relay (1.0)
hfus	33.67	kJ/mol	Joback Method
logp	3.095		Crippen Method
mcvol	199.750	ml/mol	McGowan Method
rinpol	2271.00		NIST Webbook
rinpol	2271.00		NIST Webbook
tb	634.80	K	Cheméo Relay (1.0)
tf	418.54	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307084&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point