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

Inchi: InChI=1S/C17H19NO3/c1-4-12-5-7-13(8-6-12)17(19)18-15-11-14(20-2)9-10-16(15)21-3/h
InchiKey: AXBQXNRRBAPHCZ-UHFFFAOYSA-N
Formula: C17H19NO3
SMILES: CCc1ccc(C(=O)Nc2cc(OC)ccc2OC)cc1
Mol. weight [g/mol]: 285.34

Physical Properties

Property code	Value	Unit	Source
gf	38.66	kJ/mol	Joback Method
hf	-279.11	kJ/mol	Joback Method
hfus	35.77	kJ/mol	Joback Method
hvap	77.98	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	3.518		Crippen Method
mcvol	226.160	ml/mol	McGowan Method
pc	2083.12	kPa	Joback Method
rinpol	2549.00		NIST Webbook
rinpol	2549.00		NIST Webbook
tb	805.54	K	Joback Method
tc	1032.46	K	Joback Method
tf	518.80	K	Joback Method
vc	0.849	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	650.82	J/mol×K	805.54	Joback Method
cpg	665.38	J/mol×K	843.36	Joback Method
cpg	678.74	J/mol×K	881.18	Joback Method
cpg	690.92	J/mol×K	919.00	Joback Method
cpg	701.94	J/mol×K	956.82	Joback Method
cpg	711.80	J/mol×K	994.64	Joback Method
cpg	720.55	J/mol×K	1032.46	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=U307018&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