Benzamide, N-(2,5-dimethoxyphenyl)-3-methoxy-

Inchi: InChI=1S/C16H17NO4/c1-19-12-6-4-5-11(9-12)16(18)17-14-10-13(20-2)7-8-15(14)21-3/h
InchiKey: IJHFHCBAXQOQJI-UHFFFAOYSA-N
Formula: C16H17NO4
SMILES: COc1cccc(C(=O)Nc2cc(OC)ccc2OC)c1
Mol. weight [g/mol]: 287.31

Physical Properties

Property code	Value	Unit	Source
gf	-74.76	kJ/mol	Joback Method
hf	-390.69	kJ/mol	Joback Method
hfus	34.37	kJ/mol	Joback Method
hvap	78.16	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	2.965		Crippen Method
mcvol	217.940	ml/mol	McGowan Method
pc	2241.88	kPa	Joback Method
rinpol	2555.00		NIST Webbook
rinpol	2555.00		NIST Webbook
tb	805.08	K	Joback Method
tc	1032.94	K	Joback Method
tf	529.76	K	Joback Method
vc	0.810	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.08	J/mol×K	805.08	Joback Method
cpg	635.90	J/mol×K	843.06	Joback Method
cpg	648.50	J/mol×K	881.03	Joback Method
cpg	659.87	J/mol×K	919.01	Joback Method
cpg	670.01	J/mol×K	956.99	Joback Method
cpg	678.93	J/mol×K	994.97	Joback Method
cpg	686.62	J/mol×K	1032.94	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=U306972&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