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

Inchi: InChI=1S/C16H17NO3/c1-11-5-4-6-12(9-11)16(18)17-14-10-13(19-2)7-8-15(14)20-3/h4-1

InchiKey: YTCMZASAFMOCKO-UHFFFAOYSA-N

Formula: C16H17NO3

SMILES: COc1ccc(OC)c(NC(=O)c2cccc(C)c2)c1

Mol. weight [g/mol]: 271.31

Physical Properties

Property code	Value	Unit	Source
gf	30.24	kJ/mol	Joback Method
hf	-258.47	kJ/mol	Joback Method
hfus	33.18	kJ/mol	Joback Method
hvap	75.75	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.265		Crippen Method
mcvol	212.070	ml/mol	McGowan Method
pc	2278.41	kPa	Joback Method
rinpol	2426.00		NIST Webbook
tb	782.66	K	Joback Method
tc	1012.99	K	Joback Method
tf	507.53	K	Joback Method
vc	0.792	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.59	J/mol×K	782.66	Joback Method
cpg	609.93	J/mol×K	821.05	Joback Method
cpg	623.10	J/mol×K	859.44	Joback Method
cpg	635.10	J/mol×K	897.83	Joback Method
cpg	645.96	J/mol×K	936.21	Joback Method
cpg	655.69	J/mol×K	974.60	Joback Method
cpg	664.31	J/mol×K	1012.99	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=U307117&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