

Benzamide, N-(2,5-dimethoxyphenyl)-2-bromo-

Inchi:	InChI=1S/C15H14BrNO3/c1-19-10-7-8-14(20-2)13(9-10)17-15(18)11-5-3-4-6-12(11)16/h
InchiKey:	HDXJPXBBMPRJKN-UHFFFAOYSA-N
Formula:	C15H14BrNO3
SMILES:	COc1ccc(OC)c(NC(=O)c2ccccc2Br)c1
Mol. weight [g/mol]:	336.18

Physical Properties

Property code	Value	Unit	Source
gf	36.14	kJ/mol	Joback Method
hf	-211.50	kJ/mol	Joback Method
hfus	35.88	kJ/mol	Joback Method
hvap	79.96	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	3.719		Crippen Method
mcvol	215.480	ml/mol	McGowan Method
pc	2684.64	kPa	Joback Method
rinpol	2514.00		NIST Webbook
tb	825.94	K	Joback Method
tc	1069.48	K	Joback Method
tf	556.06	K	Joback Method
vc	0.798	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.76	J/molxK	825.94	Joback Method
cpg	586.95	J/molxK	866.53	Joback Method
cpg	597.98	J/molxK	907.12	Joback Method
cpg	607.87	J/molxK	947.71	Joback Method
cpg	616.67	J/molxK	988.30	Joback Method
cpg	624.38	J/molxK	1028.89	Joback Method
cpg	631.05	J/molxK	1069.48	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=U307389&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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
r inpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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