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

Inchi: InChI=1S/C15H14BrNO3/c1-19-12-7-8-14(20-2)13(9-12)17-15(18)10-3-5-11(16)6-4-10/h
InchiKey: PFUPEKZERAFGIS-UHFFFAOYSA-N
Formula: C15H14BrNO3
SMILES: COc1ccc(OC)c(NC(=O)c2ccc(Br)cc2)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	2606.00		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/mol×K	825.94	Joback Method
cpg	586.95	J/mol×K	866.53	Joback Method
cpg	597.98	J/mol×K	907.12	Joback Method
cpg	607.87	J/mol×K	947.71	Joback Method
cpg	616.67	J/mol×K	988.30	Joback Method
cpg	624.38	J/mol×K	1028.89	Joback Method
cpg	631.05	J/mol×K	1069.48	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=U307345&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

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