Benzamide, N-(4-methoxyphenyl)-4-bromo-

Inchi: InChI=1S/C14H12BrNO2/c1-18-13-8-6-12(7-9-13)16-14(17)10-2-4-11(15)5-3-10/h2-9H,1
InchiKey: UPQBUSFVHWZAKF-UHFFFAOYSA-N
Formula: C14H12BrNO2
SMILES: COc1ccc(NC(=O)c2ccc(Br)cc2)cc1
Mol. weight [g/mol]: 306.15

Physical Properties

Property code	Value	Unit	Source
gf	142.35	kJ/mol	Joback Method
hf	-47.17	kJ/mol	Joback Method
hfus	32.49	kJ/mol	Joback Method
hvap	74.66	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	3.710		Crippen Method
mcvol	195.520	ml/mol	McGowan Method
pc	3079.57	kPa	Joback Method
rinpol	2514.00		NIST Webbook
rinpol	2514.00		NIST Webbook
tb	775.66	K	Joback Method
tc	1026.95	K	Joback Method
tf	510.04	K	Joback Method
vc	0.725	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.84	J/mol×K	775.66	Joback Method
cpg	510.24	J/mol×K	817.54	Joback Method
cpg	521.51	J/mol×K	859.42	Joback Method
cpg	531.73	J/mol×K	901.31	Joback Method
cpg	540.94	J/mol×K	943.19	Joback Method
cpg	549.22	J/mol×K	985.07	Joback Method
cpg	556.61	J/mol×K	1026.95	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=U307343&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

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