2-Bromobenzoic acid, 4-methoxyphenyl ester

Inchi: InChI=1S/C14H11BrO3/c1-17-10-6-8-11(9-7-10)18-14(16)12-4-2-3-5-13(12)15/h2-9H,1H
InchiKey: QQNKHSHHKAMKKT-UHFFFAOYSA-N
Formula: C14H11BrO3
SMILES: COc1ccc(OC(=O)c2ccccc2Br)cc1
Mol. weight [g/mol]: 307.14

Physical Properties

Property code	Value	Unit	Source
gf	-52.04	kJ/mol	Joback Method
hf	-232.86	kJ/mol	Joback Method
hfus	28.58	kJ/mol	Joback Method
hvap	70.64	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	3.677		Crippen Method
mcvol	191.410	ml/mol	McGowan Method
pc	2979.54	kPa	Joback Method
rinpol	2164.00		NIST Webbook
rinpol	2164.00		NIST Webbook
tb	747.91	K	Joback Method
tc	998.76	K	Joback Method
tf	479.61	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.39	J/mol×K	747.91	Joback Method
cpg	486.13	J/mol×K	789.72	Joback Method
cpg	497.73	J/mol×K	831.53	Joback Method
cpg	508.22	J/mol×K	873.33	Joback Method
cpg	517.63	J/mol×K	915.14	Joback Method
cpg	526.00	J/mol×K	956.95	Joback Method
cpg	533.36	J/mol×K	998.76	Joback Method
dvisc	0.0006211	Pa×s	479.61	Joback Method

dvisc	0.0004076	Pa×s	524.33	Joback Method
dvisc	0.0002858	Pa×s	569.04	Joback Method
dvisc	0.0002111	Pa×s	613.76	Joback Method
dvisc	0.0001624	Pa×s	658.48	Joback Method
dvisc	0.0001292	Pa×s	703.19	Joback Method
dvisc	0.0001057	Pa×s	747.91	Joback Method

Sources

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=U307745&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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