

3-Bromobenzoic acid, 4-methoxyphenyl ester

Inchi:	InChI=1S/C14H11BrO3/c1-17-12-5-7-13(8-6-12)18-14(16)10-3-2-4-11(15)9-10/h2-9H,1H
InchiKey:	RMTHHXJKKBLSC-UHFFFAOYSA-N
Formula:	C14H11BrO3
SMILES:	COc1ccc(OC(=O)c2ccccc(Br)c2)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	2182.00		NIST Webbook
rinpol	2182.00		NIST Webbook
tb	747.91	K	Joback Method
tc	998.76	K	Joback Method
tf	479.61	K	Joback Method
vc	0.708	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0004076	Paxs	524.33	Joback Method
dvisc	0.0002858	Paxs	569.04	Joback Method
dvisc	0.0002111	Paxs	613.76	Joback Method
dvisc	0.0001624	Paxs	658.48	Joback Method
dvisc	0.0001292	Paxs	703.19	Joback Method
dvisc	0.0001057	Paxs	747.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307551&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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