

4-Bromobenzoic acid, 2-methylphenyl ester

Inchi:	InChI=1S/C14H11BrO2/c1-10-4-2-3-5-13(10)17-14(16)11-6-8-12(15)9-7-11/h2-9H,1H3
InchiKey:	BAQANPSLAVMOTB-UHFFFAOYSA-N
Formula:	C14H11BrO2
SMILES:	Cc1ccccc1OC(=O)c1ccc(Br)cc1
Mol. weight [g/mol]:	291.14

Physical Properties

Property code	Value	Unit	Source
gf	52.96	kJ/mol	Joback Method
hf	-100.64	kJ/mol	Joback Method
hfus	27.39	kJ/mol	Joback Method
hvap	68.22	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	3.977		Crippen Method
mcvol	185.540	ml/mol	McGowan Method
pc	3035.62	kPa	Joback Method
rinpol	1968.00		NIST Webbook
rinpol	1968.00		NIST Webbook
tb	725.49	K	Joback Method
tc	980.66	K	Joback Method
tf	457.38	K	Joback Method
vc	0.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.93	J/molxK	725.49	Joback Method
cpg	503.71	J/molxK	938.13	Joback Method
cpg	494.80	J/molxK	895.60	Joback Method
cpg	484.93	J/molxK	853.07	Joback Method
cpg	474.03	J/molxK	810.55	Joback Method
cpg	462.05	J/molxK	768.02	Joback Method
cpg	511.71	J/molxK	980.66	Joback Method
dvisc	0.0001373	Paxs	725.49	Joback Method

dvisc	0.0001683	Paxs	680.81	Joback Method
dvisc	0.0002121	Paxs	636.12	Joback Method
dvisc	0.0002770	Paxs	591.43	Joback Method
dvisc	0.0003778	Paxs	546.75	Joback Method
dvisc	0.0005446	Paxs	502.06	Joback Method
dvisc	0.0008431	Paxs	457.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299027&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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