

2-Bromophenol, isoBOC

Inchi:	InChI=1S/C11H13BrO3/c1-8(2)7-14-11(13)15-10-6-4-3-5-9(10)12/h3-6,8H,7H2,1-2H3
InchiKey:	UXUIEDUKQXVYKH-UHFFFAOYSA-N
Formula:	C11H13BrO3
SMILES:	CC(C)COC(=O)Oc1ccccc1Br
Mol. weight [g/mol]:	273.12

Physical Properties

Property code	Value	Unit	Source
gf	-182.52	kJ/mol	Joback Method
hf	-401.28	kJ/mol	Joback Method
hfus	23.64	kJ/mol	Joback Method
hvap	60.63	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.620		Crippen Method
mcvol	172.900	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
rinpol	1618.00		NIST Webbook
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tb	647.17	K	Joback Method
tc	871.68	K	Joback Method
tf	391.86	K	Joback Method
vc	0.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.45	J/molxK	647.17	Joback Method
cpg	422.58	J/molxK	684.59	Joback Method
cpg	434.86	J/molxK	722.01	Joback Method
cpg	446.32	J/molxK	759.42	Joback Method
cpg	456.95	J/molxK	796.84	Joback Method
cpg	466.78	J/molxK	834.26	Joback Method
cpg	475.81	J/molxK	871.68	Joback Method
dvisc	0.0012047	Paxs	391.86	Joback Method

dvisc	0.0007054	Paxs	434.41	Joback Method
dvisc	0.0004544	Paxs	476.96	Joback Method
dvisc	0.0003146	Paxs	519.52	Joback Method
dvisc	0.0002303	Paxs	562.07	Joback Method
dvisc	0.0001761	Paxs	604.62	Joback Method
dvisc	0.0001395	Paxs	647.17	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=R235004&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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