

Phenol, 3-bromo-, acetate

Other names:	Phenol, 3-bromo-, 1-acetate 1-acetoxy-3-bromobenzene
Inchi:	InChI=1S/C8H7BrO2/c1-6(10)11-8-4-2-3-7(9)5-8/h2-5H,1H3
InchiKey:	CDLTWXBTYNNYLN-UHFFFAOYSA-N
Formula:	C8H7BrO2
SMILES:	CC(=O)Oc1cccc(Br)c1
Mol. weight [g/mol]:	215.04
CAS:	35065-86-2

Physical Properties

Property code	Value	Unit	Source
gf	-100.34	kJ/mol	Joback Method
hf	-201.86	kJ/mol	Joback Method
hfus	18.20	kJ/mol	Joback Method
hvap	51.93	kJ/mol	Joback Method
ie	8.80 ± 0.20	eV	NIST Webbook
log10ws	-2.95		Crippen Method
logp	2.374		Crippen Method
mcvol	124.760	ml/mol	McGowan Method
pc	4135.61	kPa	Joback Method
tb	556.55	K	Joback Method
tc	792.86	K	Joback Method
tf	350.82	K	Joback Method
vc	0.462	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.83	J/molxK	556.55	Joback Method
cpg	257.12	J/molxK	595.93	Joback Method
cpg	266.74	J/molxK	635.32	Joback Method
cpg	275.70	J/molxK	674.70	Joback Method
cpg	284.02	J/molxK	714.09	Joback Method
cpg	291.72	J/molxK	753.47	Joback Method

cpg	298.81	J/mol×K	792.86	Joback Method
dvisc	0.0015564	Paxs	350.82	Joback Method
dvisc	0.0010113	Paxs	385.11	Joback Method
dvisc	0.0007051	Paxs	419.40	Joback Method
dvisc	0.0005191	Paxs	453.69	Joback Method
dvisc	0.0003990	Paxs	487.97	Joback Method
dvisc	0.0003175	Paxs	522.26	Joback Method
dvisc	0.0002598	Paxs	556.55	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35065862&Units=SI

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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