

4-Bromoguaiacol, acetate

Inchi:	InChI=1S/C9H9BrO3/c1-6(11)13-8-4-3-7(10)5-9(8)12-2/h3-5H,1-2H3
InchiKey:	GCNWECQSWKBEGV-UHFFFAOYSA-N
Formula:	C9H9BrO3
SMILES:	COc1cc(Br)ccc1OC(C)=O
Mol. weight [g/mol]:	245.07

Physical Properties

Property code	Value	Unit	Source
gf	-206.55	kJ/mol	Joback Method
hf	-366.19	kJ/mol	Joback Method
hfus	21.59	kJ/mol	Joback Method
hvap	57.23	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.383		Crippen Method
mvol	144.720	ml/mol	McGowan Method
pc	3530.46	kPa	Joback Method
rinpol	1527.10		NIST Webbook
rinpol	1527.10		NIST Webbook
tb	606.83	K	Joback Method
tc	836.24	K	Joback Method
tf	396.84	K	Joback Method
vc	0.535	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.32	J/molxK	606.83	Joback Method
cpg	360.78	J/molxK	798.01	Joback Method
cpg	352.39	J/molxK	759.77	Joback Method
cpg	343.34	J/molxK	721.54	Joback Method
cpg	333.64	J/molxK	683.30	Joback Method
cpg	323.30	J/molxK	645.07	Joback Method
cpg	368.52	J/molxK	836.24	Joback Method
dvisc	0.0001847	Paxs	606.83	Joback Method

dvisc	0.0002229	Paxs	571.83	Joback Method
dvisc	0.0002757	Paxs	536.83	Joback Method
dvisc	0.0003512	Paxs	501.84	Joback Method
dvisc	0.0004639	Paxs	466.84	Joback Method
dvisc	0.0006412	Paxs	431.84	Joback Method
dvisc	0.0009382	Paxs	396.84	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=U352875&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
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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