

2-(Acetyloxy)-5-bromobenzoic acid

Inchi:	InChI=1S/C9H7BrO4/c1-5(11)14-8-3-2-6(10)4-7(8)9(12)13/h2-4H,1H3,(H,12,13)
InchiKey:	VRJBEVQGGJOSGOX-UHFFFAOYSA-N
Formula:	C9H7BrO4
SMILES:	CC(=O)Oc1ccc(Br)cc1C(=O)O
Mol. weight [g/mol]:	259.05
CAS:	1503-53-3

Physical Properties

Property code	Value	Unit	Source
gf	-367.29	kJ/mol	Joback Method
hf	-498.78	kJ/mol	Joback Method
hfus	26.09	kJ/mol	Joback Method
hvap	78.24	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.073		Crippen Method
mcvol	146.290	ml/mol	McGowan Method
pc	4379.97	kPa	Joback Method
tb	730.46	K	Joback Method
tc	951.00	K	Joback Method
tf	485.36	K	Joback Method
vc	0.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.38	J/mol×K	730.46	Joback Method
cpg	372.55	J/mol×K	914.24	Joback Method
cpg	367.04	J/mol×K	877.49	Joback Method
cpg	360.98	J/mol×K	840.73	Joback Method
cpg	354.36	J/mol×K	803.97	Joback Method
cpg	347.16	J/mol×K	767.22	Joback Method
cpg	377.51	J/mol×K	951.00	Joback Method
dvisc	0.0000533	Pa×s	730.46	Joback Method
dvisc	0.0000720	Pa×s	689.61	Joback Method

dvisc	0.0001010	Pa×s	648.76	Joback Method
dvisc	0.0001483	Pa×s	607.91	Joback Method
dvisc	0.0002302	Pa×s	567.06	Joback Method
dvisc	0.0003824	Pa×s	526.21	Joback Method
dvisc	0.0006919	Pa×s	485.36	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C1503533&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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