3-Bromo-4-methoxybenzaldehyde

Other names: Benzaldehyde, 3-bromo-4-methoxy-
p-Anisaldehyde, 3-bromo-
3-Bromo-p-anisaldehyde
Inchi: InChI=1S/C8H7BrO2/c1-11-8-3-2-6(5-10)4-7(8)9/h2-5H,1H3
InchiKey: QMPNFQLVIGPNEI-UHFFFAOYSA-N
Formula: C8H7BrO2
SMILES: COc1ccc(C=O)cc1Br
Mol. weight [g/mol]: 215.04
CAS: 34841-06-0

Physical Properties

Property code	Value	Unit	Source
gf	-80.57	kJ/mol	Joback Method
hf	-186.33	kJ/mol	Joback Method
hfus	18.50	kJ/mol	Joback Method
hvap	52.57	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.270		Crippen Method
mcvol	124.760	ml/mol	McGowan Method
pc	4114.41	kPa	Joback Method
tb	556.32	K	Joback Method
tc	788.01	K	Joback Method
tf	355.41	K	Joback Method
vc	0.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.43	J/mol×K	556.32	Joback Method
cpg	290.09	J/mol×K	749.39	Joback Method
cpg	282.68	J/mol×K	710.78	Joback Method
cpg	274.72	J/mol×K	672.16	Joback Method
cpg	266.20	J/mol×K	633.55	Joback Method
cpg	257.11	J/mol×K	594.93	Joback Method

cpg	296.97	J/mol×K	788.01	Joback Method
dvisc	0.0002769	Pa×s	556.32	Joback Method
dvisc	0.0003327	Pa×s	522.83	Joback Method
dvisc	0.0004099	Pa×s	489.35	Joback Method
dvisc	0.0005208	Pa×s	455.87	Joback Method
dvisc	0.0006871	Pa×s	422.38	Joback Method
dvisc	0.0009510	Pa×s	388.89	Joback Method
dvisc	0.0013992	Pa×s	355.41	Joback Method

Sources

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=C34841060&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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