

5-Bromo-2-ethoxybenzaldehyde

Inchi:	InChI=1S/C9H9BrO2/c1-2-12-9-4-3-8(10)5-7(9)6-11/h3-6H,2H2,1H3
InchiKey:	NFCBVQSSJAXEJD-UHFFFAOYSA-N
Formula:	C9H9BrO2
SMILES:	CCOc1ccc(Br)cc1C=O
Mol. weight [g/mol]:	229.07
CAS:	79636-94-5

Physical Properties

Property code	Value	Unit	Source
gf	-72.15	kJ/mol	Joback Method
hf	-206.97	kJ/mol	Joback Method
hfus	21.09	kJ/mol	Joback Method
hvap	54.79	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	2.660		Crippen Method
mcvol	138.850	ml/mol	McGowan Method
pc	3650.93	kPa	Joback Method
tb	579.20	K	Joback Method
tc	806.45	K	Joback Method
tf	366.68	K	Joback Method
vc	0.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.41	J/molxK	579.20	Joback Method
cpg	302.18	J/molxK	617.07	Joback Method
cpg	312.31	J/molxK	654.95	Joback Method
cpg	321.80	J/molxK	692.82	Joback Method
cpg	330.67	J/molxK	730.70	Joback Method
cpg	338.95	J/molxK	768.57	Joback Method
cpg	346.64	J/molxK	806.45	Joback Method
dvisc	0.0013758	Paxs	366.68	Joback Method
dvisc	0.0009171	Paxs	402.10	Joback Method

dvisc	0.0006528	Paxs	437.52	Joback Method
dvisc	0.0004890	Paxs	472.94	Joback Method
dvisc	0.0003813	Paxs	508.36	Joback Method
dvisc	0.0003071	Paxs	543.78	Joback Method
dvisc	0.0002540	Paxs	579.20	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=C79636945&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/22-756-8/5-Bromo-2-ethoxybenzaldehyde.pdf>

Generated by Cheméo on 2024-04-28 20:28:05.95474477 +0000 UTC m=+16625334.875322092.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.