3,4-Ethylenedioxybromobenzene

Other names:	1,4-Benzodioxin, 6-bromo-2,3-dihydro- 6-bromo-2,3-dihydro-1,4-benzodioxin
Inchi:	InChI=1S/C8H7BrO2/c9-6-1-2-7-8(5-6)11-4-3-10-7/h1-2,5H,3-4H2
InchiKey:	LFCURAJBHDNUNG-UHFFFAOYSA-N
Formula:	C8H7BrO2
SMILES:	Brc1ccc2c(c1)OCCO2
Mol. weight [g/mol]:	215.04
CAS:	52287-51-1

Physical Properties

Property code	Value	Unit	Source
gf	8.07	kJ/mol	Joback Method
hf	-145.55	kJ/mol	Joback Method
hfus	25.95	kJ/mol	Joback Method
hvap	52.85	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	2.220		Crippen Method
mcvol	118.200	ml/mol	McGowan Method
pc	4782.59	kPa	Joback Method
tb	554.82	K	Joback Method
tc	809.14	K	Joback Method
tf	362.98	K	Joback Method
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.55	J/mol×K	554.82	Joback Method
cpg	295.77	J/mol×K	766.75	Joback Method
cpg	287.74	J/mol×K	724.37	Joback Method
cpg	278.99	J/mol×K	681.98	Joback Method
cpg	269.42	J/mol×K	639.59	Joback Method
cpg	258.97	J/mol×K	597.21	Joback Method
cpg	303.14	J/mol×K	809.14	Joback Method

dvisc	0.0004456	Pa×s	554.82	Joback Method
dvisc	0.0005361	Pa×s	522.85	Joback Method
dvisc	0.0006608	Pa×s	490.87	Joback Method
dvisc	0.0008386	Pa×s	458.90	Joback Method
dvisc	0.0011028	Pa×s	426.93	Joback Method
dvisc	0.0015161	Pa×s	394.95	Joback Method
dvisc	0.0022044	Pa×s	362.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52287511&Units=SI
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

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