

2-Bromomethyl-2,3-dihydrobenzofuran

Inchi:	InChI=1S/C9H9BrO/c10-6-8-5-7-3-1-2-4-9(7)11-8/h1-4,8H,5-6H2
InchiKey:	QYFBYHXEEODTMX-UHFFFAOYSA-N
Formula:	C9H9BrO
SMILES:	BrCC1Cc2ccccc2O1
Mol. weight [g/mol]:	213.07
CAS:	19997-53-6

Physical Properties

Property code	Value	Unit	Source
gf	116.63	kJ/mol	Joback Method
hf	-36.90	kJ/mol	Joback Method
hfus	24.12	kJ/mol	Joback Method
hvap	49.42	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.385		Crippen Method
mcvol	126.420	ml/mol	McGowan Method
pc	4026.13	kPa	Joback Method
tb	536.83	K	Joback Method
tc	778.66	K	Joback Method
tf	334.44	K	Joback Method
vc	0.471	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.29	J/mol×K	536.83	Joback Method
cpg	280.36	J/mol×K	577.13	Joback Method
cpg	292.37	J/mol×K	617.44	Joback Method
cpg	303.41	J/mol×K	657.74	Joback Method
cpg	313.57	J/mol×K	698.05	Joback Method
cpg	322.94	J/mol×K	738.35	Joback Method
cpg	331.59	J/mol×K	778.66	Joback Method
dvisc	0.0021015	Paxs	334.44	Joback Method
dvisc	0.0015396	Paxs	368.17	Joback Method

dvisc	0.0011884	Paxs	401.90	Joback Method
dvisc	0.0009548	Paxs	435.63	Joback Method
dvisc	0.0007916	Paxs	469.37	Joback Method
dvisc	0.0006731	Paxs	503.10	Joback Method
dvisc	0.0005841	Paxs	536.83	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=C19997536&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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