Benzene, (1-bromoethyl)-, (R)-

Inchi: InChI=1S/C8H9Br/c1-7(9)8-5-3-2-4-6-8/h2-7H,1H3/t7-/m0/s1
InchiKey: CRRUGYDDEMGVDY-ZETCQYMHSA-N
Formula: C8H9Br
SMILES: CC(Br)c1ccccc1
Mol. weight [g/mol]: 185.06
CAS: 1459-14-9

Physical Properties

Property code	Value	Unit	Source
gf	140.77	kJ/mol	Joback Method
hf	49.13	kJ/mol	Joback Method
hfus	12.28	kJ/mol	Joback Method
hvap	41.73	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	3.143		Crippen Method
mcvol	117.320	ml/mol	McGowan Method
pc	4015.93	kPa	Joback Method
tb	476.20	K	NIST Webbook
tc	708.92	K	Joback Method
tf	251.14	K	Joback Method
vc	0.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.09	J/mol×K	474.84	Joback Method
cpg	225.68	J/mol×K	513.85	Joback Method
cpg	237.36	J/mol×K	552.87	Joback Method
cpg	248.20	J/mol×K	591.88	Joback Method
cpg	258.23	J/mol×K	630.89	Joback Method
cpg	267.51	J/mol×K	669.90	Joback Method
cpg	276.09	J/mol×K	708.92	Joback Method
dvisc	0.0041027	Pa×s	251.14	Joback Method
dvisc	0.0019756	Pa×s	288.42	Joback Method

dvisc	0.0011246	Pa×s	325.71	Joback Method
dvisc	0.0007187	Pa×s	362.99	Joback Method
dvisc	0.0004993	Pa×s	400.27	Joback Method
dvisc	0.0003690	Pa×s	437.56	Joback Method
dvisc	0.0002860	Pa×s	474.84	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	360.20	K	2.00	NIST Webbook

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=C1459149&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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume