Benzene, (3-bromopropyl)-

Other names:	(3-Bromopropyl)benzene
	(«gamma»-Bromopropyl)benzene
	(Â«gammaÂ»-Bromopropyl)benzene
	1-Bromo-3-phenylpropane
	1-Phenyl-3-bromopropane
	3-Bromo-1-phenylpropane
	3-Phenylpropyl bromide
	NSC 133438
	«gamma»-Phenylpropyl bromide
	Â«gammaÂ»-Phenylpropyl bromide
Inchi:	InChI=1S/C9H11Br/c10-8-4-7-9-5-2-1-3-6-9/h1-3,5-6H,4,7-8H2
InchiKey:	XMZQWZJMTBCUFT-UHFFFAOYSA-N
Formula:	C9H11Br
SMILES:	BrCCCc1ccccc1
Mol. weight [g/mol]:	199.09
CAS:	637-59-2

Physical Properties

Property code	Value	Unit	Source
gf	151.63	kJ/mol	Joback Method
hf	33.77	kJ/mol	Joback Method
hfus	18.39	kJ/mol	Joback Method
hvap	44.34	kJ/mol	Joback Method
ie	9.00 ± 0.10	eV	NIST Webbook
log10ws	-3.12		Crippen Method
logp	3.014		Crippen Method
mcvol	131.410	ml/mol	McGowan Method
pc	3534.66	kPa	Joback Method
tb	492.70	K	NIST Webbook
tb	493.00	K	NIST Webbook
tc	722.79	K	Joback Method
tf	277.41	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.71	J/mol×K	498.16	Joback Method
cpg	312.76	J/mol×K	685.35	Joback Method
cpg	302.74	J/mol×K	647.92	Joback Method
cpg	291.97	J/mol×K	610.48	Joback Method
cpg	280.41	J/mol×K	573.04	Joback Method
cpg	268.00	J/mol×K	535.60	Joback Method
cpg	322.08	J/mol×K	722.79	Joback Method
dvisc	0.0002807	Pa×s	498.16	Joback Method
dvisc	0.0003555	Pa×s	461.37	Joback Method
dvisc	0.0004691	Pa×s	424.58	Joback Method
dvisc	0.0006524	Pa×s	387.78	Joback Method
dvisc	0.0009723	Pa×s	350.99	Joback Method
dvisc	0.0015910	Pa×s	314.20	Joback Method
dvisc	0.0029667	Pa×s	277.41	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41219e+01
Coeff. B	-3.94294e+03
Coeff. C	-7.81070e+01
Temperature range (K), min.	363.12
Temperature range (K), max.	525.64

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=C637592&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume