Benzene, 1-(bromomethyl)-2-methyl-

Other names:	1-(Bromomethyl)-2-methylbenzene
	2-(Bromomethyl)toluene
	2-Methylbenzyl bromide
	2-Xylyl bromide
	NSC 60145
	o-(Bromomethyl)toluene
	o-Methylbenzyl bromide
	o-Xylene, «alpha»-bromo-
	o-Xylene, Â«alphaÂ»-bromo-
	o-Xylyl bromide
	«alpha»-Bromo-o-xylene
	«alpha»-Bromo-ortho-xylene
	Â«alphaÂ»-Bromo-o-xylene
	Â«alphaÂ»-Bromo-ortho-xylene
Inchi:	InChI=1S/C8H9Br/c1-7-4-2-3-5-8(7)6-9/h2-5H,6H2,1H3
InchiKey:	WGVYCXYGPNNUQA-UHFFFAOYSA-N
Formula:	C8H9Br
SMILES:	Cc1ccccc1CBr
Mol. weight [g/mol]:	185.06
CAS:	89-92-9

Physical Properties

Property code	Value	Unit	Source
gf	133.58	kJ/mol	Joback Method
hf	42.94	kJ/mol	Joback Method
hfus	15.41	kJ/mol	Joback Method
hvap	42.78	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	2.890		Crippen Method
mcvol	117.320	ml/mol	McGowan Method
pc	3901.37	kPa	Joback Method
tb	480.26	K	Joback Method
tc	710.10	K	Joback Method
tf	278.66	K	Joback Method
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.97	J/mol×K	480.26	Joback Method
cpg	224.69	J/mol×K	518.57	Joback Method
cpg	235.65	J/mol×K	556.87	Joback Method
cpg	245.87	J/mol×K	595.18	Joback Method
cpg	255.40	J/mol×K	633.48	Joback Method
cpg	264.29	J/mol×K	671.79	Joback Method
cpg	272.56	J/mol×K	710.10	Joback Method
dvisc	0.0021418	Pa×s	278.66	Joback Method
dvisc	0.0012813	Pa×s	312.26	Joback Method
dvisc	0.0008469	Pa×s	345.86	Joback Method
dvisc	0.0006024	Pa×s	379.46	Joback Method
dvisc	0.0004529	Pa×s	413.06	Joback Method
dvisc	0.0003554	Pa×s	446.66	Joback Method
dvisc	0.0002886	Pa×s	480.26	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	489.70	K	98.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40783e+01
Coeff. B	-3.91255e+03
Coeff. C	-7.74120e+01
Temperature range (K), min.	361.12
Temperature range (K), max.	523.70

Sources

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
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=C89929&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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume