

Benzene, 1-(bromomethyl)-4-methyl-

Other names:	1-(Bromomethyl)-4-methylbenzene 4-(Bromomethyl)toluene 4-Methylbenzyl bromide NSC 8050 p-(Bromomethyl)toluene p-Methylbenzyl bromide p-Xylene, «alpha»-bromo- p-Xylene, Â«alphaÂ»-bromo- p-Xylyl bromide p-Xylyl-«alpha»-bromide p-Xylyl-Â«alphaÂ»-bromide «alpha»-Bromo-p-xylene «alpha»-Bromo-p-xylol Â«alphaÂ»-Bromo-p-xylene Â«alphaÂ»-Bromo-p-xylol
Inchi:	InChI=1S/C8H9Br/c1-7-2-4-8(6-9)5-3-7/h2-5H,6H2,1H3
InchiKey:	WZRKSPFYXUXINF-UHFFFAOYSA-N
Formula:	C8H9Br
SMILES:	<chem>Cc1ccc(CBr)cc1</chem>
Mol. weight [g/mol]:	185.06
CAS:	104-81-4

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	492.20	K	NIST Webbook
tc	710.10	K	Joback Method
tf	307.15 ± 1.50	K	NIST Webbook
vc	0.438	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	492.20	K	98.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.42193e+01
Coeff. B	-3.97434e+03
Coeff. C	-7.82460e+01
Temperature range (K), min.	363.52
Temperature range (K), max.	524.41

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C104814&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
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
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

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