2-CHLOROBENZYL BROMIDE

Other names:	o-Chlorobenzyl bromide
	2-Chlorobenzyl bromide
	Toluene, «alpha»-bromo-o-chloro-
	1-(bromomethyl)-2-chlorobenzene
Inchi:	InChI=1S/C7H6BrCl/c8-5-6-3-1-2-4-7(6)9/h1-4H,5H2
InchiKey:	PURSZYWBIQIANP-UHFFFAOYSA-N
Formula:	C7H6BrCl
SMILES:	Clc1ccccc1CBr
Mol. weight [g/mol]:	205.48

Physical Properties

Property code	Value	Unit	Source
af	0.4081		Cheméo Relay (1.0)
gf	113.23	kJ/mol	Joback Method
hf	32.83	kJ/mol	Cheméo Relay (1.0)
hfus	17.02	kJ/mol	Joback Method
hvap	57.91	kJ/mol	Cheméo Relay (1.0)
ie	9.06	eV	Cheméo Relay (1.0)
log10ws	-3.30		Cheméo Relay (1.0)
logp	3.235		Crippen Method
mcvol	115.470	ml/mol	McGowan Method
pc	4205.63	kPa	Joback Method
rinpol	1237.00		NIST Webbook
rinpol	1237.00		NIST Webbook
tb	508.87	K	Cheméo Relay (1.0)
tc	728.29	K	Cheméo Relay (1.0)
tf	311.29	K	Cheméo Relay (1.0)
vc	0.409	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.64	J/mol×K	494.81	Joback Method
cpg	205.32	J/mol×K	534.77	Joback Method

cpg	214.28	J/mol×K	574.72	Joback Method
cpg	222.55	J/mol×K	614.68	Joback Method
cpg	230.19	J/mol×K	654.64	Joback Method
cpg	237.24	J/mol×K	694.60	Joback Method
cpg	243.74	J/mol×K	734.55	Joback Method
dvisc	0.0020778	Pa×s	297.31	Joback Method
dvisc	0.0012960	Pa×s	330.23	Joback Method
dvisc	0.0008806	Pa×s	363.14	Joback Method
dvisc	0.0006381	Pa×s	396.06	Joback Method
dvisc	0.0004857	Pa×s	428.98	Joback Method
dvisc	0.0003844	Pa×s	461.89	Joback Method
dvisc	0.0003139	Pa×s	494.81	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	376.70	K	1.30	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C611176&Units=SI

Legend

af: Acentric Factor
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume