

Benzene, 2-(bromomethyl)-1,3-dichloro-

Other names:	«alpha»-Bromo-2,6-dichlorotoluene 2,6-Dichlorobenzyl bromide Toluene, «alpha»-bromo-2,6-dichloro- alpha-bromo-2,6-dichlorotoluene
Inchi:	InChI=1S/C7H5BrCl2/c8-4-5-6(9)2-1-3-7(5)10/h1-3H,4H2
InchiKey:	PDFGFQUSSYSWNI-UHFFFAOYSA-N
Formula:	C7H5BrCl2
SMILES:	Clc1cccc(Cl)c1CBr
Mol. weight [g/mol]:	239.93
CAS:	20443-98-5

Physical Properties

Property code	Value	Unit	Source
gf	91.67	kJ/mol	Joback Method
hf	20.63	kJ/mol	Joback Method
hfus	20.83	kJ/mol	Joback Method
hvap	49.98	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.888		Crippen Method
mcvol	127.710	ml/mol	McGowan Method
pc	3935.71	kPa	Joback Method
tb	537.22	K	Joback Method
tc	783.23	K	Joback Method
tf	339.75	K	Joback Method
vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.76	J/molxK	537.22	Joback Method
cpg	252.20	J/molxK	742.22	Joback Method
cpg	246.04	J/molxK	701.22	Joback Method
cpg	239.36	J/molxK	660.22	Joback Method
cpg	232.12	J/molxK	619.22	Joback Method

cpg	224.26	J/mol×K	578.22	Joback Method
cpg	257.87	J/mol×K	783.23	Joback Method
dvisc	0.0002997	Paxs	537.22	Joback Method
dvisc	0.0003609	Paxs	504.31	Joback Method
dvisc	0.0004459	Paxs	471.40	Joback Method
dvisc	0.0005687	Paxs	438.49	Joback Method
dvisc	0.0007545	Paxs	405.57	Joback Method
dvisc	0.0010523	Paxs	372.66	Joback Method
dvisc	0.0015654	Paxs	339.75	Joback Method

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=C20443985&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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