3-Chlorobenzal bromide

Other names: Benzene, 1-chloro-3-(dibromomethyl)-
Toluene, m-chloro-alpha,alpha-dibromo-
1-chloro-3-(dibromomethyl)benzene
Inchi: InChI=1S/C7H5Br2Cl/c8-7(9)5-2-1-3-6(10)4-5/h1-4,7H
InchiKey: GXTJYNIKOLTVNC-UHFFFAOYSA-N
Formula: C7H5Br2Cl
SMILES: Clc1cccc(C(Br)Br)c1
Mol. weight [g/mol]: 284.38
CAS: 70288-97-0

Physical Properties

Property code	Value	Unit	Source
gf	125.11	kJ/mol	Joback Method
hf	68.89	kJ/mol	Joback Method
hfus	18.78	kJ/mol	Joback Method
hvap	50.98	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	4.128		Crippen Method
mcvol	132.970	ml/mol	McGowan Method
pc	4659.34	kPa	Joback Method
tb	560.53	K	Joback Method
tc	822.28	K	Joback Method
tf	342.11	K	Joback Method
vc	0.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.88	J/mol×K	560.53	Joback Method
cpg	261.81	J/mol×K	778.66	Joback Method
cpg	255.78	J/mol×K	735.03	Joback Method
cpg	249.14	J/mol×K	691.41	Joback Method
cpg	241.83	J/mol×K	647.78	Joback Method
cpg	233.77	J/mol×K	604.16	Joback Method

cpg	267.32	J/mol×K	822.28	Joback Method
dvisc	0.0002883	Pa×s	560.53	Joback Method
dvisc	0.0003572	Pa×s	524.13	Joback Method
dvisc	0.0004570	Pa×s	487.72	Joback Method
dvisc	0.0006085	Pa×s	451.32	Joback Method
dvisc	0.0008518	Pa×s	414.92	Joback Method
dvisc	0.0012721	Pa×s	378.51	Joback Method
dvisc	0.0020692	Pa×s	342.11	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C70288970&Units=SI
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume