Benzene, (1-bromo-3,3,3-trichloropropyl)

Inchi: InChI=1S/C9H8BrCl3/c10-8(6-9(11,12)13)7-4-2-1-3-5-7/h1-5,8H,6H2
InchiKey: GYXDKVQPLSJHKZ-UHFFFAOYSA-N
Formula: C9H8BrCl3
SMILES: ClC(Cl)(Cl)CC(Br)c1ccccc1
Mol. weight [g/mol]: 302.42

Physical Properties

Property code	Value	Unit	Source
gf	116.24	kJ/mol	Joback Method
hf	-27.48	kJ/mol	Joback Method
hfus	20.05	kJ/mol	Joback Method
hvap	55.81	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	4.883		Crippen Method
mcvol	168.130	ml/mol	McGowan Method
pc	3206.41	kPa	Joback Method
rinpol	1618.00		NIST Webbook
rinpol	1618.00		NIST Webbook
tb	606.78	K	Joback Method
tc	865.67	K	Joback Method
tf	354.59	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.69	J/mol×K	606.78	Joback Method
cpg	376.46	J/mol×K	822.52	Joback Method
cpg	369.13	J/mol×K	779.38	Joback Method
cpg	361.00	J/mol×K	736.23	Joback Method
cpg	351.97	J/mol×K	693.08	Joback Method
cpg	341.91	J/mol×K	649.93	Joback Method
cpg	383.14	J/mol×K	865.67	Joback Method
dvisc	0.0001965	Pa×s	606.78	Joback Method

dvisc	0.0002596	Pa×s	564.75	Joback Method
dvisc	0.0003585	Pa×s	522.72	Joback Method
dvisc	0.0005240	Pa×s	480.69	Joback Method
dvisc	0.0008236	Pa×s	438.65	Joback Method
dvisc	0.0014246	Pa×s	396.62	Joback Method
dvisc	0.0028062	Pa×s	354.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R515043&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume