Alpha,alpha,alpha,alpha',alpha',alpha'-2-heptachl

Other names: Benzene, 1-chloro-2,5-bis(trichloromethyl)-
Inchi: InChI=1S/C8H3Cl7/c9-6-3-4(7(10,11)12)1-2-5(6)8(13,14)15/h1-3H
InchiKey: URRUNMMSCQPLOQ-UHFFFAOYSA-N
Formula: C8H3Cl7
SMILES: Clc1cc(C(Cl)(Cl)Cl)ccc1C(Cl)(Cl)Cl
Mol. weight [g/mol]: 347.28
CAS: 10388-10-0

Physical Properties

Property code	Value	Unit	Source
gf	31.80	kJ/mol	Joback Method
hf	-122.54	kJ/mol	Joback Method
hfus	24.29	kJ/mol	Joback Method
hvap	65.11	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	5.993		Crippen Method
mcvol	185.500	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
tb	674.63	K	Joback Method
tc	951.31	K	Joback Method
tf	445.66	K	Joback Method
vc	0.697	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.26	J/mol×K	674.63	Joback Method
cpg	341.96	J/mol×K	720.74	Joback Method
cpg	347.72	J/mol×K	766.86	Joback Method
cpg	352.71	J/mol×K	812.97	Joback Method
cpg	357.09	J/mol×K	859.09	Joback Method
cpg	361.01	J/mol×K	905.20	Joback Method
cpg	364.62	J/mol×K	951.31	Joback Method
dvisc	0.0011097	Pa×s	445.66	Joback Method

dvisc	0.0006912	Pa×s	483.82	Joback Method
dvisc	0.0004614	Pa×s	521.98	Joback Method
dvisc	0.0003254	Pa×s	560.14	Joback Method
dvisc	0.0002400	Pa×s	598.31	Joback Method
dvisc	0.0001835	Pa×s	636.47	Joback Method
dvisc	0.0001447	Pa×s	674.63	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10388100&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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