Chlorbenside

Other names:	Benzene, 1-chloro-4-[[(4-chlorophenyl)methyl]thio]-
	Sulfide, p-chlorobenzyl p-chlorophenyl
	p-Chlorobenzyl p-chlorophenyl sulfide
	p-Chlorobenzyl p-chlorophenyl sulphide
	Chloracid
	Chlorbensid (German)
	Chlorbenzide
	Chlorocid
	Chlorparacide
	Chlorsulphacide
	CP 20
	Mitox
	4-Chlorobenzyl 4-Chlorophenyl sulfide
	(4-Chloor-benzyl)-(4-chloor-fenyl)-sulfide
	(4-Chlor-benzyl)-(4-chlor-phenyl)-sulfid
	(4-Cloro-benzil)-(4-cloro-fenil)-solfuro
	p,p'-Dichlorodiphenyl sulfide
	Chloorbenzide
	Chlorbensid
	Chlorbenxide
	Chlorocide
	Chloroparacide
	Chlorosulfacide
	ENT 20,696
	HRS 860
	RD 2195
	Sulfure de 4-chlorobenzyle et de 4-chlorophenyle
	1-Chloro-4-(((4-chlorophenyl)methyl)thio)benzene
	4-Chlorobenzyl 4-chlorophenyl sulphide
	4-Chlorophenyl 4'-chlorobenzyl sulfide
	Chlorobenside
	NSC 33078
Inchi:	InChI=1S/C13H10Cl2S/c14-11-3-1-10(2-4-11)9-16-13-7-5-12(15)6-8-13/h1-8H,9H2
InchiKey:	ZHLKXBJTJHRTTE-UHFFFAOYSA-N
Formula:	C13H10Cl2S
SMILES:	Clc1ccc(CSc2ccc(Cl)cc2)cc1
Mol. weight [g/mol]:	269.19
CAS:	103-17-3

Physical Properties

Property code	Value	Unit	Source
gf	273.40	kJ/mol	Joback Method
hf	148.86	kJ/mol	Joback Method
hfus	29.25	kJ/mol	Joback Method
hvap	66.00	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	5.286		Crippen Method
mcvol	187.340	ml/mol	McGowan Method
pc	2796.51	kPa	Joback Method
rinpol	2045.00		NIST Webbook
rinpol	2045.00		NIST Webbook
rinpol	2040.00		NIST Webbook
tb	703.80	K	Joback Method
tc	974.79	K	Joback Method
tf	343.80 ± 0.20	K	NIST Webbook
tf	344.50 ± 0.20	K	NIST Webbook
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.71	J/mol×K	703.80	Joback Method
cpg	437.01	J/mol×K	748.96	Joback Method
cpg	449.04	J/mol×K	794.13	Joback Method
cpg	459.89	J/mol×K	839.29	Joback Method
cpg	469.63	J/mol×K	884.46	Joback Method
cpg	478.34	J/mol×K	929.62	Joback Method
cpg	486.08	J/mol×K	974.79	Joback Method
hfust	32.22	kJ/mol	343.80	NIST Webbook
hfust	32.22	kJ/mol	343.80	NIST Webbook
sfust	96.55	J/mol×K	343.80	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103173&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume