

Benzene, 1,1'-[sulfonylbis(methylene)]bis[4-chloro-

Other names:

Bis[4-chlorobenzyl]sulfone

Bis(p-chlorobenzyl) sulfone

Inchi: InChI=1S/C14H12Cl2O2S/c15-13-5-1-11(2-6-13)9-19(17,18)10-12-3-7-14(16)8-4-12/h1-14

InchiKey: JEVYVLLSVHNREX-UHFFFAOYSA-N

Formula: C14H12Cl2O2S

SMILES: O=S(=O)(Cc1ccc(Cl)cc1)Cc1ccc(Cl)cc1

Mol. weight [g/mol]: 315.21

CAS: 84355-05-5

Physical Properties

Property code	Value	Unit	Source
gf	-219.84	kJ/mol	Joback Method
hf	-367.00	kJ/mol	Joback Method
hfus	39.09	kJ/mol	Joback Method
hvap	80.04	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	4.108		Crippen Method
mcvol	213.170	ml/mol	McGowan Method
pc	2925.00	kPa	Joback Method
tb	705.68	K	Joback Method
tc	942.17	K	Joback Method
tf	423.82	K	Joback Method
vc	0.828	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.96	J/mol×K	705.68	Joback Method
cpg	522.74	J/mol×K	745.09	Joback Method
cpg	535.30	J/mol×K	784.51	Joback Method
cpg	546.69	J/mol×K	823.92	Joback Method
cpg	556.94	J/mol×K	863.34	Joback Method
cpg	566.09	J/mol×K	902.75	Joback Method
cpg	574.19	J/mol×K	942.17	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=C84355055&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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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