Benzyl phenyl sulfone

Other names:	Benzene, [(phenylmethyl)sulfonyl]-
	Sulfone, benzyl phenyl
	Benzyl phenyl sulphone
	[(phenylmethyl)sulphonyl]benzene
Inchi:	InChI=1S/C13H12O2S/c14-16(15,13-9-5-2-6-10-13)11-12-7-3-1-4-8-12/h1-10H,11H2
InchiKey:	FABCMLOTUSCWOR-UHFFFAOYSA-N
Formula:	C13H12O2S
SMILES:	O=S(=O)(Cc1ccccc1)c1ccccc1
Mol. weight [g/mol]:	232.30
CAS:	3112-88-7

Physical Properties

Property code	Value	Unit	Source
gf	-185.14	kJ/mol	Joback Method
hf	-291.94	kJ/mol	Joback Method
hfus	28.89	kJ/mol	Joback Method
hvap	67.72	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	2.660		Crippen Method
mcvol	174.600	ml/mol	McGowan Method
pc	3677.55	kPa	Joback Method
tb	597.98	K	Joback Method
tc	831.51	K	Joback Method
tf	420.00 ± 3.00	K	NIST Webbook
vc	0.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.85	J/mol×K	597.98	Joback Method
cpg	424.39	J/mol×K	636.90	Joback Method
cpg	439.62	J/mol×K	675.82	Joback Method
cpg	453.60	J/mol×K	714.74	Joback Method
cpg	466.38	J/mol×K	753.67	Joback Method

cpg	477.99	J/mol×K	792.59	Joback Method
cpg	488.48	J/mol×K	831.51	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=C3112887&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