Benzyl sulfone

Other names:	Dibenzyl sulfone
	Benzene, 1,1'-[sulfonylbis(methylene)]bis-
	Dibenzyl sulphone
Inchi:	InChI=1S/C14H14O2S/c15-17(16,11-13-7-3-1-4-8-13)12-14-9-5-2-6-10-14/h1-10H,11-12
InchiKey:	AWHNUHMUCGRKRA-UHFFFAOYSA-N
Formula:	C14H14O2S
SMILES:	O=S(=O)(Cc1ccccc1)Cc1ccccc1
Mol. weight [g/mol]:	246.32
CAS:	620-32-6

Physical Properties

Property code	Value	Unit	Source
chs	-7829.60 ± 1.00	kJ/mol	NIST Webbook
gf	-176.72	kJ/mol	Joback Method
hf	-157.10 ± 3.20	kJ/mol	NIST Webbook
hfs	-282.60 ± 1.20	kJ/mol	NIST Webbook
hfus	31.48	kJ/mol	Joback Method
hsub	114.00 ± 2.00	kJ/mol	NIST Webbook
hvap	69.95	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	2.802		Crippen Method
mcvol	188.690	ml/mol	McGowan Method
pc	3284.05	kPa	Joback Method
tb	620.86	K	Joback Method
tc	849.79	K	Joback Method
tf	425.00 ± 3.00	K	NIST Webbook
tf	422.70 ± 1.00	K	NIST Webbook
tf	425.00 ± 3.00	K	NIST Webbook
tf	402.00 ± 2.00	K	NIST Webbook
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	457.68	J/mol×K	620.86	Joback Method
cpg	474.68	J/mol×K	659.01	Joback Method
cpg	490.36	J/mol×K	697.17	Joback Method
cpg	504.77	J/mol×K	735.32	Joback Method
cpg	517.96	J/mol×K	773.48	Joback Method
cpg	529.98	J/mol×K	811.63	Joback Method
cpg	540.88	J/mol×K	849.79	Joback Method

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=C620326&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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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