

p-(Methylthio)benzyl alcohol

Other names:	4-(Methylthio)benzyl alcohol Benzenemethanol, 4-(methylthio)- [4-(Methylsulfanyl)phenyl]methanol
Inchi:	InChI=1S/C8H10OS/c1-10-8-4-2-7(6-9)3-5-8/h2-5,9H,6H2,1H3
InchiKey:	MTXQKSQYMREAGJ-UHFFFAOYSA-N
Formula:	C8H10OS
SMILES:	CSc1ccc(CO)cc1
Mol. weight [g/mol]:	154.23
CAS:	3446-90-0

Physical Properties

Property code	Value	Unit	Source
gf	15.56	kJ/mol	Joback Method
hf	-93.75	kJ/mol	Joback Method
hfus	18.35	kJ/mol	Joback Method
hvap	59.84	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	1.901		Crippen Method
mcvol	122.040	ml/mol	McGowan Method
pc	4103.88	kPa	Joback Method
rinpol	1419.00		NIST Webbook
rinpol	1419.00		NIST Webbook
tb	575.06	K	Joback Method
tc	792.59	K	Joback Method
tf	314.08	K	Joback Method
vc	0.449	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.63	J/mol×K	575.06	Joback Method
cpg	279.16	J/mol×K	611.32	Joback Method
cpg	289.05	J/mol×K	647.57	Joback Method
cpg	298.32	J/mol×K	683.83	Joback Method

cpg	306.99	J/mol×K	720.08	Joback Method
cpg	315.07	J/mol×K	756.34	Joback Method
cpg	322.60	J/mol×K	792.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3446900&Units=SI
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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