4-(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

Physical Properties

Property code	Value	Unit	Source
hf	-112.21	kJ/mol	Cheméo Relay (1.0)
hfus	18.35	kJ/mol	Joback Method
hvap	85.95	kJ/mol	Cheméo Relay (1.0)
ie	8.08	eV	Cheméo Relay (1.0)
log10ws	-1.83		Cheméo Relay (1.0)
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	539.96	K	Cheméo Relay (1.0)
tc	772.53	K	Cheméo Relay (1.0)
tf	321.11	K	Cheméo Relay (1.0)

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3446900&Units=SI

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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