o-Mercaptobenzyl alcohol

Inchi: InChI=1S/C7H8OS/c8-5-6-3-1-2-4-7(6)9/h1-4,8-9H,5H2
InchiKey: FYWFCRHZXORPFH-UHFFFAOYSA-N
Formula: C7H8OS
SMILES: OCc1ccccc1S
Mol. weight [g/mol]: 140.21

Physical Properties

Property code	Value	Unit	Source
hfus	15.67	kJ/mol	Joback Method
ie	8.39	eV	Cheméo Relay (1.0)
log10ws	-1.65		Cheméo Relay (1.0)
logp	1.468		Crippen Method
mcvol	107.950	ml/mol	McGowan Method
tb	536.70	K	Cheméo Relay (1.0)
tf	335.23	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.09	J/mol×K	546.26	Joback Method
cpg	232.47	J/mol×K	583.23	Joback Method
cpg	241.25	J/mol×K	620.21	Joback Method
cpg	249.45	J/mol×K	657.18	Joback Method
cpg	257.11	J/mol×K	694.15	Joback Method
cpg	264.24	J/mol×K	731.13	Joback Method
cpg	270.88	J/mol×K	768.10	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=C4521317&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point