2,6-Dimethylbenzenethiol, S-acetyl-

Inchi: InChI=1S/C10H12OS/c1-7-5-4-6-8(2)10(7)12-9(3)11/h4-6H,1-3H3
InchiKey: UWFDUOBIXFDFCT-UHFFFAOYSA-N
Formula: C10H12OS
SMILES: CC(=O)Sc1c(C)cccc1C
Mol. weight [g/mol]: 180.27

Physical Properties

Property code	Value	Unit	Source
gf	30.67	kJ/mol	Joback Method
hf	-106.85	kJ/mol	Joback Method
hfus	20.65	kJ/mol	Joback Method
hvap	55.02	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	2.942		Crippen Method
mcvol	145.920	ml/mol	McGowan Method
pc	3096.73	kPa	Joback Method
rinpol	1420.70		NIST Webbook
tb	587.49	K	Joback Method
tc	824.42	K	Joback Method
tf	338.25	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.62	J/mol×K	587.49	Joback Method
cpg	339.00	J/mol×K	626.98	Joback Method
cpg	351.54	J/mol×K	666.47	Joback Method
cpg	363.26	J/mol×K	705.96	Joback Method
cpg	374.16	J/mol×K	745.45	Joback Method
cpg	384.28	J/mol×K	784.94	Joback Method
cpg	393.62	J/mol×K	824.42	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=U353021&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
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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