4-Isopropylbenzenethiol, S-methyl-

Inchi: InChI=1S/C10H14S/c1-8(2)9-4-6-10(11-3)7-5-9/h4-8H,1-3H3
InchiKey: IGKRCEMLHDKLEE-UHFFFAOYSA-N
Formula: C10H14S
SMILES: CSc1ccc(C(C)C)cc1
Mol. weight [g/mol]: 166.28

Physical Properties

Property code	Value	Unit	Source
gf	166.78	kJ/mol	Joback Method
hf	11.92	kJ/mol	Joback Method
hfus	15.92	kJ/mol	Joback Method
hvap	47.22	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	3.532		Crippen Method
mcvol	144.350	ml/mol	McGowan Method
pc	2963.34	kPa	Joback Method
rinpol	1371.70		NIST Webbook
rinpol	1371.70		NIST Webbook
tb	528.20	K	Joback Method
tc	761.14	K	Joback Method
tf	260.80	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.01	J/mol×K	528.20	Joback Method
cpg	325.47	J/mol×K	567.02	Joback Method
cpg	339.98	J/mol×K	605.85	Joback Method
cpg	353.59	J/mol×K	644.67	Joback Method
cpg	366.32	J/mol×K	683.50	Joback Method
cpg	378.20	J/mol×K	722.32	Joback Method
cpg	389.25	J/mol×K	761.14	Joback Method

Sources

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=U353048&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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