2-Isopropylbenzenethiol, S-methyl-

Inchi: InChI=1S/C10H14S/c1-8(2)9-6-4-5-7-10(9)11-3/h4-8H,1-3H3
InchiKey: UWRWHOKKUJISAM-UHFFFAOYSA-N
Formula: C10H14S
SMILES: CSc1ccccc1C(C)C
Mol. weight [g/mol]: 166.28

Physical Properties

Property code	Value	Unit	Source
hf	4.68	kJ/mol	Cheméo Relay (1.0)
hfus	15.92	kJ/mol	Joback Method
hvap	62.31	kJ/mol	Cheméo Relay (1.0)
ie	7.99	eV	Cheméo Relay (1.0)
log10ws	-4.15		Cheméo Relay (1.0)
logp	3.532		Crippen Method
mcvol	144.350	ml/mol	McGowan Method
pc	2963.34	kPa	Joback Method
rinpol	1329.00		NIST Webbook
tb	506.33	K	Cheméo Relay (1.0)
tc	708.33	K	Cheméo Relay (1.0)
tf	261.67	K	Cheméo Relay (1.0)
vc	0.508	m3/kmol	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-7.89000e+00
Coeff. B	8.15750e-01
Coeff. C	-4.47360e-04
Coeff. D	8.03000e-08
Coeff. E	0.00000e+00
Basis	predicted

Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

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=U353043&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
vc:	Critical Volume

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