2-ISOPROPYLBENZENETHIOL

Inchi: InChI=1S/C9H12S/c1-7(2)8-5-3-4-6-9(8)10/h3-7,10H,1-2H3
InchiKey: QEDRUXIMTJVXFL-UHFFFAOYSA-N
Formula: C9H12S
SMILES: CC(C)c1ccccc1S
Mol. weight [g/mol]: 152.26
CAS: 6262-87-9

Physical Properties

Property code	Value	Unit	Source
af	0.3504		Cheméo Relay (1.0)
gf	154.63	kJ/mol	Joback Method
hf	19.52	kJ/mol	Cheméo Relay (1.0)
hfus	13.24	kJ/mol	Joback Method
hvap	60.01	kJ/mol	Cheméo Relay (1.0)
ie	8.01	eV	Cheméo Relay (1.0)
log10ws	-3.83		Cheméo Relay (1.0)
logp	3.099		Crippen Method
mcvol	130.260	ml/mol	McGowan Method
pc	3484.76	kPa	Joback Method
rinpol	1237.40		NIST Webbook
tb	493.20	K	NIST Webbook
tc	710.11	K	Cheméo Relay (1.0)
tf	271.99	K	Cheméo Relay (1.0)
vc	0.445	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.72	J/mol×K	499.40	Joback Method
cpg	278.10	J/mol×K	539.04	Joback Method
cpg	291.56	J/mol×K	578.68	Joback Method
cpg	304.15	J/mol×K	618.33	Joback Method
cpg	315.90	J/mol×K	657.97	Joback Method
cpg	326.85	J/mol×K	697.61	Joback Method

cpg	337.03	J/mol×K	737.25	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46434e+01
Coeff. B	-4.15994e+03
Coeff. C	-7.82460e+01
Temperature range (K), min.	368.02
Temperature range (K), max.	524.02

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6262879&Units=SI

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):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af: Acentric Factor

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

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume