

1-Naphthalenethiol

Other names:	«alpha»-Naphthyl mercaptan «alpha»-Thionaphthol 1-Mercaptonaphthalene 1-Naphthyl mercaptan 1-Thionaphthol naphthalene-1-thiol
Inchi:	InChI=1S/C10H8S/c11-10-7-3-5-8-4-1-2-6-9(8)10/h1-7,11H
InchiKey:	SEXOVMIIVBKGGM-UHFFFAOYSA-N
Formula:	C10H8S
SMILES:	Sc1cccc2ccccc12
Mol. weight [g/mol]:	160.24
CAS:	529-36-2

Physical Properties

Property code	Value	Unit	Source
gf	272.14	kJ/mol	Joback Method
hf	204.88	kJ/mol	Joback Method
hfus	16.37	kJ/mol	Joback Method
hvap	49.17	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.128		Crippen Method
mcvol	124.890	ml/mol	McGowan Method
pc	4146.27	kPa	Joback Method
ripol	2131.00		NIST Webbook
tb	541.70	K	Joback Method
tc	804.80	K	Joback Method
tf	310.56	K	Joback Method
vc	0.464	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.32	J/mol×K	541.70	Joback Method
cpg	267.46	J/mol×K	585.55	Joback Method

cpg	279.44	J/mol×K	629.40	Joback Method
cpg	290.37	J/mol×K	673.25	Joback Method
cpg	300.33	J/mol×K	717.10	Joback Method
cpg	309.44	J/mol×K	760.95	Joback Method
cpg	317.78	J/mol×K	804.80	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C529362&Units=SI

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
hvac:	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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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