3-Cyclohexene-1-methanethiol, «alpha»,«alpha»,4-trimethyl-

Other names: 1-p-menthene-8-thiol
1-p-menthen-8-thiol
p-1-menthene-8-thiol
1- p-menth-1-ene-8-thiol
p-1-menthen-8-thiol
p-Menth-1-ene-8-thiol
«alpha»,«alpha»,4-trimethylcyclohex-3-ene-1-methanethiol

Inchi: InChI=1S/C10H18S/c1-8-4-6-9(7-5-8)10(2,3)11/h4,9,11H,5-7H2,1-3H3

InchiKey: ZQPCOAKGRYBBMR-UHFFFAOYSA-N

Formula: C10H18S

SMILES: CC1=CCC(C(C)(C)S)CC1

Mol. weight [g/mol]: 170.31

CAS: 71159-90-5

Physical Properties

Property code	Value	Unit	Source
gf	110.33	kJ/mol	Joback Method
hf	-119.37	kJ/mol	Joback Method
hfus	10.95	kJ/mol	Joback Method
hvap	44.68	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	3.441		Crippen Method
mcvol	152.950	ml/mol	McGowan Method
pc	2862.74	kPa	Joback Method
rinpol	1291.00		NIST Webbook
rinpol	1283.00		NIST Webbook
rinpol	1283.00		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1264.00		NIST Webbook
rinpol	1281.00		NIST Webbook
ripol	1619.00		NIST Webbook
ripol	1598.00		NIST Webbook
ripol	1615.00		NIST Webbook
ripol	1598.00		NIST Webbook
ripol	1598.00		NIST Webbook
ripol	1598.00		NIST Webbook

tb	511.52	K	Joback Method
tc	748.85	K	Joback Method
tf	262.00	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.36	J/mol×K	511.52	Joback Method
cpg	366.17	J/mol×K	551.08	Joback Method
cpg	384.64	J/mol×K	590.63	Joback Method
cpg	401.83	J/mol×K	630.19	Joback Method
cpg	417.82	J/mol×K	669.74	Joback Method
cpg	432.66	J/mol×K	709.30	Joback Method
cpg	446.42	J/mol×K	748.85	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C71159905&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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