1-p-menthene-8-thiol

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]:	170.32

Physical Properties

Property code	Value	Unit	Source
hf	-54.60	kJ/mol	Cheméo Relay (1.0)
hfus	10.95	kJ/mol	Joback Method
hvap	55.21	kJ/mol	Cheméo Relay (1.0)
ie	8.14	eV	Cheméo Relay (1.0)
log10ws	-3.66		Cheméo Relay (1.0)
logp	3.441		Crippen Method
mcvol	152.950	ml/mol	McGowan Method
rinpol	1291.00		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1281.00		NIST Webbook
rinpol	1264.00		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1283.00		NIST Webbook
rinpol	1283.00		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1264.00		NIST Webbook
ripol	1619.00		NIST Webbook
ripol	1598.00		NIST Webbook
ripol	1598.00		NIST Webbook
ripol	1598.00		NIST Webbook
ripol	1615.00		NIST Webbook

ripol	1598.00		NIST Webbook
ripol	1615.00		NIST Webbook
ripol	1598.00		NIST Webbook
tb	484.94	K	Cheméo Relay (1.0)
tf	272.79	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C71159905&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

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point