Cyclohexanone, 2-(1-mercapto-1-methylethyl)-5-methyl-, trans-

Other names:	p-Menthon-8-thiol, trans
	5-Methyl-2-(1-methyl-1-sulfanylethyl)cyclohexanone, trans
	p-Menthan-3-one, 8-mercapto, trans
	trans-2-(1-Mercapto-1-methylethyl)-5-methylcyclohexan-1-one
	Trans-8-mercapto-3-Methanone
Inchi:	InChI=1S/C10H18OS/c1-7-4-5-8(9(11)6-7)10(2,3)12/h7-8,12H,4-6H2,1-3H3
InchiKey:	RVOKNSFEAOYULQ-UHFFFAOYSA-N
Formula:	C10H18OS
SMILES:	CC1CCC(C(C)(C)S)C(=O)C1
Mol. weight [g/mol]:	186.31
CAS:	33281-91-3

Physical Properties

Property code	Value	Unit	Source
gf	-40.30	kJ/mol	Joback Method
hf	-323.72	kJ/mol	Joback Method
hfus	10.70	kJ/mol	Joback Method
hvap	47.66	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.700		Crippen Method
mcvol	158.820	ml/mol	McGowan Method
pc	2805.41	kPa	Joback Method
ripol	1859.00		NIST Webbook
tb	570.53	K	Joback Method
tc	819.75	K	Joback Method
tf	312.70	K	Joback Method
vc	0.578	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.58	J/mol×K	570.53	Joback Method
cpg	420.51	J/mol×K	612.07	Joback Method
cpg	440.08	J/mol×K	653.60	Joback Method

cpg	458.30	J/mol×K	695.14	Joback Method
cpg	475.19	J/mol×K	736.68	Joback Method
cpg	490.78	J/mol×K	778.21	Joback Method
cpg	505.09	J/mol×K	819.75	Joback Method

Sources

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=C33281913&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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