S-(2-((1R,4S)-4-methyl-2-oxocyclohexyl)propan-2-ethanethioate, ref-

InchI: InChI=1S/C12H20O2S/c1-8-5-6-10(11(14)7-8)12(3,4)15-9(2)13/h8,10H,5-7H2,1-4H3
InchiKey: AMXPURQVAMENCC-UHFFFAOYSA-N
Formula: C12H20O2S
SMILES: CC(=O)SC(C)(C)C1CCC(C)CC1=O
Mol. weight [g/mol]: 228.35
CAS: 166022-16-8

Physical Properties

Property code	Value	Unit	Source
gf	-148.65	kJ/mol	Joback Method
hf	-474.19	kJ/mol	Joback Method
hfus	17.57	kJ/mol	Joback Method
hvap	58.94	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	3.050		Crippen Method
mcvol	188.570	ml/mol	McGowan Method
pc	2347.36	kPa	Joback Method
rinpol	1603.50		NIST Webbook
rinpol	1603.50		NIST Webbook
tb	676.08	K	Joback Method
tc	920.33	K	Joback Method
tf	383.11	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	529.37	J/mol×K	676.08	Joback Method
cpg	549.14	J/mol×K	716.79	Joback Method
cpg	567.42	J/mol×K	757.50	Joback Method
cpg	584.23	J/mol×K	798.20	Joback Method
cpg	599.59	J/mol×K	838.91	Joback Method
cpg	613.50	J/mol×K	879.62	Joback Method
cpg	625.99	J/mol×K	920.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C166022168&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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