

S-(2-((1R,4R)-4-Methyl-2-oxocyclohexyl)propan-2-yl)ethanethioate

InChI: CC(=O)SC(C)(C)C1CCC(C)CC1=O

InChIKey: AMXPURQVAMENCC-PSASIEDQSA-N

Formula: C12H20O2S

SMILES: CC(=O)SC(C)(C)C1CCC(C)CC1=O

Mol. weight [g/mol]: 228.35

CAS: 166022-17-9

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	1589.40		NIST Webbook
rinpol	1589.40		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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C166022179&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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