2-isopropyl-thiacyclopentane

Inchi: InChI=1S/C7H14S/c1-6(2)7-4-3-5-8-7/h6-7H,3-5H2,1-2H3
InchiKey: GONQWPIOWIVQPT-UHFFFAOYSA-N
Formula: C7H14S
SMILES: CC(C)C1CCCS1
Mol. weight [g/mol]: 130.25

Physical Properties

Property code	Value	Unit	Source
gf	82.03	kJ/mol	Joback Method
hf	-87.35	kJ/mol	Joback Method
hfus	7.96	kJ/mol	Joback Method
hvap	36.86	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	2.538		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	3427.87	kPa	Joback Method
rinpol	1014.00		NIST Webbook
rinpol	1014.00		NIST Webbook
tb	422.23	K	Joback Method
tc	638.07	K	Joback Method
tf	248.00	K	Joback Method
vc	0.408	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.53	J/mol×K	422.23	Joback Method
cpg	237.53	J/mol×K	458.20	Joback Method
cpg	252.65	J/mol×K	494.18	Joback Method
cpg	266.92	J/mol×K	530.15	Joback Method
cpg	280.37	J/mol×K	566.12	Joback Method
cpg	293.04	J/mol×K	602.10	Joback Method
cpg	304.96	J/mol×K	638.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R208661&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