Thiophane, propyl-

Other names:	2-propyl-thiacyclopentane
	2-Propyl-thiolane
	Thiolane, 2-propyl
	Thiophene, 2-propyltetrahydro
	Thiophene, tetrahydro, 2-propyl
Inchi:	InChI=1S/C7H14S/c1-2-4-7-5-3-6-8-7/h7H,2-6H2,1H3
InchiKey:	RKTPCTKFTDSWND-UHFFFAOYSA-N
Formula:	C7H14S
SMILES:	CCCC1CCCS1
Mol. weight [g/mol]:	130.25
CAS:	1551-34-4

Physical Properties

Property code	Value	Unit	Source
gf	84.47	kJ/mol	Joback Method
hf	-82.07	kJ/mol	Joback Method
hfus	11.48	kJ/mol	Joback Method
hvap	37.25	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.682		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	3395.98	kPa	Joback Method
rinpol	1037.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1017.00		NIST Webbook
rinpol	1013.00		NIST Webbook
rinpol	1017.00		NIST Webbook
rinpol	1021.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1071.00		NIST Webbook
rinpol	1077.00		NIST Webbook
rinpol	1028.00		NIST Webbook
rinpol	1028.00		NIST Webbook
rinpol	1028.00		NIST Webbook
rinpol	1037.00		NIST Webbook
rinpol	1013.00		NIST Webbook
tb	422.67	K	Joback Method

tc	633.29	K	Joback Method
tf	263.00	K	Joback Method
vc	0.414	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.52	J/mol×K	422.67	Joback Method
cpg	237.04	J/mol×K	457.77	Joback Method
cpg	251.72	J/mol×K	492.88	Joback Method
cpg	265.60	J/mol×K	527.98	Joback Method
cpg	278.72	J/mol×K	563.08	Joback Method
cpg	291.09	J/mol×K	598.18	Joback Method
cpg	302.76	J/mol×K	633.29	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1551344&Units=SI

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