2-n-Propylthiane

Other names:	2-Propyltetrahydro-2H-thiopyran
	2-Propyl-thiacyclohexane
	Thiane, 2-propyl
	2-Propylthiane
	2-Propylthiapyran
Inchi:	InChI=1S/C8H16S/c1-2-5-8-6-3-4-7-9-8/h8H,2-7H2,1H3
InchiKey:	QNLNFNXMMCOGFT-UHFFFAOYSA-N
Formula:	C8H16S
SMILES:	CCCC1CCCCS1
Mol. weight [g/mol]:	144.28
CAS:	17912-23-1

Physical Properties

Property code	Value	Unit	Source
gf	80.79	kJ/mol	Joback Method
hf	-108.87	kJ/mol	Joback Method
hfus	11.97	kJ/mol	Joback Method
hvap	39.64	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	3.072		Crippen Method
mcvol	129.070	ml/mol	McGowan Method
pc	3131.49	kPa	Joback Method
rinpol	1117.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	1108.00		NIST Webbook
tb	449.82	K	Joback Method
tc	666.35	K	Joback Method
tf	270.75	K	Joback Method
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.72	J/mol×K	449.82	Joback Method
cpg	280.38	J/mol×K	485.91	Joback Method
cpg	297.10	J/mol×K	522.00	Joback Method
cpg	312.90	J/mol×K	558.08	Joback Method
cpg	327.82	J/mol×K	594.17	Joback Method
cpg	341.89	J/mol×K	630.26	Joback Method
cpg	355.12	J/mol×K	666.35	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17912231&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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