2-propyl-1,3-dithiolane

Inchi: InChI=1S/C6H12S2/c1-2-3-6-7-4-5-8-6/h6H,2-5H2,1H3
InchiKey: YFPNQWYEDBOBMI-UHFFFAOYSA-N
Formula: C6H12S2
SMILES: CCCC1SCCS1
Mol. weight [g/mol]: 148.29

Physical Properties

Property code	Value	Unit	Source
gf	115.91	kJ/mol	Joback Method
hf	-16.17	kJ/mol	Joback Method
hfus	12.54	kJ/mol	Joback Method
hvap	40.83	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.593		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	3782.33	kPa	Joback Method
rinpol	1229.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1222.00		NIST Webbook
rinpol	1188.00		NIST Webbook
rinpol	1188.00		NIST Webbook
rinpol	1222.00		NIST Webbook
rinpol	1244.00		NIST Webbook
rinpol	1223.00		NIST Webbook
rinpol	1188.00		NIST Webbook
rinpol	1202.00		NIST Webbook
rinpol	1176.00		NIST Webbook
tb	447.62	K	Joback Method
tc	677.09	K	Joback Method
tf	335.18	K	Joback Method
vc	0.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.17	J/mol×K	447.62	Joback Method
cpg	240.50	J/mol×K	485.86	Joback Method
cpg	253.96	J/mol×K	524.11	Joback Method
cpg	266.60	J/mol×K	562.35	Joback Method
cpg	278.45	J/mol×K	600.60	Joback Method
cpg	289.55	J/mol×K	638.84	Joback Method
cpg	299.94	J/mol×K	677.09	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R78880&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

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