1-(propylthio)propyl propyl disulfide

Other names: 6-Ethyl-4,5,7-trithiadecane
Inchi: InChI=1S/C9H20S3/c1-4-7-10-9(6-3)12-11-8-5-2/h9H,4-8H2,1-3H3
InchiKey: NPIXBDUKSDQMKL-UHFFFAOYSA-N
Formula: C9H20S3
SMILES: CCCSSC(CC)SCCC
Mol. weight [g/mol]: 224.45

Physical Properties

Property code	Value	Unit	Source
gf	121.82	kJ/mol	Joback Method
hf	-108.76	kJ/mol	Joback Method
hfus	27.93	kJ/mol	Joback Method
hvap	55.69	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.657		Crippen Method
mcvol	186.720	ml/mol	McGowan Method
pc	2443.48	kPa	Joback Method
rinpol	1557.00		NIST Webbook
rinpol	1535.90		NIST Webbook
rinpol	1557.00		NIST Webbook
rinpol	1535.90		NIST Webbook
tb	611.22	K	Joback Method
tc	836.59	K	Joback Method
tf	279.39	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.82	J/mol×K	611.22	Joback Method
cpg	458.74	J/mol×K	648.78	Joback Method
cpg	473.75	J/mol×K	686.34	Joback Method
cpg	487.85	J/mol×K	723.91	Joback Method
cpg	501.05	J/mol×K	761.47	Joback Method

cpg	513.34	J/mol×K	799.03	Joback Method
cpg	524.73	J/mol×K	836.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R56777&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