1-Methyl-2-(1-(propylthio)propyl)disulfane

Inchi: InChI=1S/C7H16S3/c1-4-6-9-7(5-2)10-8-3/h7H,4-6H2,1-3H3
InchiKey: QCPKKCRPPOQHIG-UHFFFAOYSA-N
Formula: C7H16S3
SMILES: CCCSC(CC)SSC
Mol. weight [g/mol]: 196.41

Physical Properties

Property code	Value	Unit	Source
hfus	22.75	kJ/mol	Joback Method
hvap	63.36	kJ/mol	Cheméo Relay (1.0)
logp	3.877		Crippen Method
mcvol	158.540	ml/mol	McGowan Method
rinpol	1379.00		NIST Webbook
rinpol	1395.00		NIST Webbook
rinpol	1395.00		NIST Webbook
rinpol	1421.50		NIST Webbook
rinpol	1421.50		NIST Webbook
rinpol	1379.00		NIST Webbook
tb	516.78	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.04	J/mol×K	565.46	Joback Method
cpg	361.34	J/mol×K	604.52	Joback Method
cpg	374.85	J/mol×K	643.58	Joback Method
cpg	387.56	J/mol×K	682.64	Joback Method
cpg	399.47	J/mol×K	721.70	Joback Method
cpg	410.57	J/mol×K	760.76	Joback Method
cpg	420.86	J/mol×K	799.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C126876219&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature