1-(1-PROPENYLTHIO)PROPANE

Inchi: InChI=1S/C6H12S/c1-3-5-7-6-4-2/h3,5H,4,6H2,1-2H3/b5-3+
InchiKey: RKVNNVDQIVWRNA-HWKANZROSA-N
Formula: C6H12S
SMILES: C/C=C/SCCC
Mol. weight [g/mol]: 116.23

Physical Properties

Property code	Value	Unit	Source
hfus	15.63	kJ/mol	Joback Method
logp	2.663		Crippen Method
mcvol	107.450	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.21	J/mol×K	409.62	Joback Method
cpg	202.37	J/mol×K	442.74	Joback Method
cpg	213.00	J/mol×K	475.87	Joback Method
cpg	223.11	J/mol×K	508.99	Joback Method
cpg	232.74	J/mol×K	542.11	Joback Method
cpg	241.89	J/mol×K	575.24	Joback Method
cpg	250.59	J/mol×K	608.36	Joback Method

Sources

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):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C33922702&Units=SI
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
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume