(E)-Prop-1-en-1-yl propanedithioate

Inchi: InChI=1S/C6H10S2/c1-3-5-8-6(7)4-2/h3,5H,4H2,1-2H3/b5-3+
InchiKey: HGWSQZSABMPVRF-HWKANZROSA-N
Formula: C6H10S2
SMILES: CC=CSC(=S)CC
Mol. weight [g/mol]: 146.27
CAS: 67269-06-1

Physical Properties

Property code	Value	Unit	Source
gf	230.04	kJ/mol	Joback Method
hf	138.42	kJ/mol	Joback Method
hfus	20.23	kJ/mol	Joback Method
hvap	42.45	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	2.991		Crippen Method
mcvol	119.500	ml/mol	McGowan Method
pc	3749.97	kPa	Joback Method
rinpol	1164.60		NIST Webbook
rinpol	1164.60		NIST Webbook
tb	479.66	K	Joback Method
tc	708.66	K	Joback Method
tf	220.97	K	Joback Method
vc	0.442	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.21	J/mol×K	479.66	Joback Method
cpg	231.85	J/mol×K	517.83	Joback Method
cpg	241.71	J/mol×K	555.99	Joback Method
cpg	250.84	J/mol×K	594.16	Joback Method
cpg	259.32	J/mol×K	632.33	Joback Method
cpg	267.21	J/mol×K	670.49	Joback Method
cpg	274.57	J/mol×K	708.66	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C67269061&Units=SI

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