3-Ethyl-1,2-dithi-5-ene

Inchi: InChI=1S/C6H10S2/c1-2-6-4-3-5-7-8-6/h3,5-6H,2,4H2,1H3
InchiKey: YUYZREYFRPXMSZ-UHFFFAOYSA-N
Formula: C6H10S2
SMILES: CCC1CC=CSS1
Mol. weight [g/mol]: 146.27

Physical Properties

Property code	Value	Unit	Source
gf	133.77	kJ/mol	Joback Method
hf	35.45	kJ/mol	Joback Method
hfus	11.67	kJ/mol	Joback Method
hvap	41.30	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	3.064		Crippen Method
mcvol	112.940	ml/mol	McGowan Method
pc	4082.92	kPa	Joback Method
rinpol	1117.00		NIST Webbook
tb	451.05	K	Joback Method
tc	692.78	K	Joback Method
tf	332.42	K	Joback Method
vc	0.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	210.23	J/mol×K	451.05	Joback Method
cpg	224.13	J/mol×K	491.34	Joback Method
cpg	237.14	J/mol×K	531.63	Joback Method
cpg	249.31	J/mol×K	571.91	Joback Method
cpg	260.65	J/mol×K	612.20	Joback Method
cpg	271.22	J/mol×K	652.49	Joback Method
cpg	281.04	J/mol×K	692.78	Joback Method

Sources

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=R261395&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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