2-Ethyl[1,3]dithiane

Other names: 1,3-Dithiane, 2-ethyl
Inchi: InChI=1S/C6H12S2/c1-2-6-7-4-3-5-8-6/h6H,2-5H2,1H3
InchiKey: MMCSAFCIQDJGDY-UHFFFAOYSA-N
Formula: C6H12S2
SMILES: CCC1SCCCS1
Mol. weight [g/mol]: 148.29
CAS: 6007-23-4

Physical Properties

Property code	Value	Unit	Source
gf	103.81	kJ/mol	Joback Method
hf	-22.33	kJ/mol	Joback Method
hfus	10.44	kJ/mol	Joback Method
hvap	41.00	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.593		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	3901.37	kPa	Joback Method
rinpol	1131.00		NIST Webbook
rinpol	1129.00		NIST Webbook
rinpol	1131.00		NIST Webbook
tb	451.89	K	Joback Method
tc	690.97	K	Joback Method
tf	331.66	K	Joback Method
vc	0.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.07	J/mol×K	451.89	Joback Method
cpg	240.44	J/mol×K	491.74	Joback Method
cpg	254.89	J/mol×K	531.58	Joback Method
cpg	268.45	J/mol×K	571.43	Joback Method
cpg	281.14	J/mol×K	611.28	Joback Method

cpg	293.01	J/mol×K	651.12	Joback Method
cpg	304.08	J/mol×K	690.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6007234&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

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