2-Ethylidene[1,3]dithiane

Inchi: InChI=1S/C6H10S2/c1-2-6-7-4-3-5-8-6/h2H,3-5H2,1H3
InchiKey: WNNFMNLZTIEHOD-UHFFFAOYSA-N
Formula: C6H10S2
SMILES: CC=C1SCCCS1
Mol. weight [g/mol]: 146.27
CAS: 51102-62-6

Physical Properties

Property code	Value	Unit	Source
gf	156.98	kJ/mol	Joback Method
hf	74.04	kJ/mol	Joback Method
hfus	9.70	kJ/mol	Joback Method
hvap	42.10	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.718		Crippen Method
mcvol	112.940	ml/mol	McGowan Method
pc	4222.04	kPa	Joback Method
ripol	1778.00		NIST Webbook
tb	463.20	K	Joback Method
tc	711.70	K	Joback Method
tf	346.26	K	Joback Method
vc	0.381	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.83	J/mol×K	463.20	Joback Method
cpg	222.29	J/mol×K	504.62	Joback Method
cpg	234.83	J/mol×K	546.03	Joback Method
cpg	246.50	J/mol×K	587.45	Joback Method
cpg	257.35	J/mol×K	628.87	Joback Method
cpg	267.43	J/mol×K	670.29	Joback Method
cpg	276.78	J/mol×K	711.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51102626&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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