2-Octyl-2,3-dehydro-1,4-dithiane

Inchi: InChI=1S/C12H22S2/c1-2-3-4-5-6-7-8-12-11-13-9-10-14-12/h9-10,12H,2-8,11H2,1H3
InchiKey: GIIHRUNWMSFEQZ-UHFFFAOYSA-N
Formula: C12H22S2
SMILES: CCCCCCCCC1CSC=CS1
Mol. weight [g/mol]: 230.43

Physical Properties

Property code	Value	Unit	Source
gf	184.29	kJ/mol	Joback Method
hf	-88.39	kJ/mol	Joback Method
hfus	27.21	kJ/mol	Joback Method
hvap	54.65	kJ/mol	Joback Method
log10ws	-5.46		Crippen Method
logp	5.057		Crippen Method
mcvol	197.480	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
rinpol	1801.00		NIST Webbook
tb	588.33	K	Joback Method
tc	805.33	K	Joback Method
tf	400.04	K	Joback Method
vc	0.719	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.48	J/mol×K	588.33	Joback Method
cpg	504.56	J/mol×K	624.50	Joback Method
cpg	522.52	J/mol×K	660.66	Joback Method
cpg	539.40	J/mol×K	696.83	Joback Method
cpg	555.25	J/mol×K	733.00	Joback Method
cpg	570.12	J/mol×K	769.16	Joback Method
cpg	584.04	J/mol×K	805.33	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=R391149&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