

2-Ethyl-1,3-dithiolane

Inchi: InChI=1S/C5H10S2/c1-2-5-6-3-4-7-5/h5H,2-4H2,1H3
InchiKey: QBBPWAMFOHAOHM-UHFFFAOYSA-N
Formula: C5H10S2
SMILES: CCC1SCCS1
Mol. weight [g/mol]: 134.26

Physical Properties

Property code	Value	Unit	Source
gf	107.49	kJ/mol	Joback Method
hf	4.47	kJ/mol	Joback Method
hfus	9.95	kJ/mol	Joback Method
hvap	38.61	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	2.202		Crippen Method
mcvol	103.150	ml/mol	McGowan Method
pc	4271.86	kPa	Joback Method
rinpol	1128.00		NIST Webbook
rinpol	1129.00		NIST Webbook
rinpol	1148.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1095.00		NIST Webbook
tb	424.74	K	Joback Method
tc	657.67	K	Joback Method
tf	323.91	K	Joback Method
vc	0.348	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.62	J/mol×K	424.74	Joback Method
cpg	199.62	J/mol×K	463.56	Joback Method
cpg	211.82	J/mol×K	502.38	Joback Method
cpg	223.25	J/mol×K	541.21	Joback Method
cpg	233.96	J/mol×K	580.03	Joback Method
cpg	243.97	J/mol×K	618.85	Joback Method
cpg	253.32	J/mol×K	657.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R78812&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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