2-ethyl-4-methyl-1,3-dithiolane

Inchi: InChI=1S/C6H12S2/c1-3-6-7-4-5(2)8-6/h5-6H,3-4H2,1-2H3
InchiKey: PYBVIKJOGRMFFA-UHFFFAOYSA-N
Formula: C6H12S2
SMILES: CCC1SCC(C)S1
Mol. weight [g/mol]: 148.29

Physical Properties

Property code	Value	Unit	Source
gf	108.20	kJ/mol	Joback Method
hf	-36.51	kJ/mol	Joback Method
hfus	13.62	kJ/mol	Joback Method
hvap	40.52	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.591		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	3633.35	kPa	Joback Method
rinpol	1153.00		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1156.00		NIST Webbook
tb	442.95	K	Joback Method
tc	672.12	K	Joback Method
tf	330.94	K	Joback Method
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.98	J/mol×K	442.95	Joback Method

cpg	241.66	J/mol×K	481.14	Joback Method
cpg	255.51	J/mol×K	519.34	Joback Method
cpg	268.56	J/mol×K	557.53	Joback Method
cpg	280.84	J/mol×K	595.73	Joback Method
cpg	292.39	J/mol×K	633.92	Joback Method
cpg	303.23	J/mol×K	672.12	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R78830&Units=SI

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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