2-Ethyl-2-methyl-1,3-dithiolane

Other names: 1,3-Dithiolane, 2-ethyl-2-methyl-
2-Methyl-2-ethyl-1,3-dithiolane
Inchi: InChI=1S/C6H12S2/c1-3-6(2)7-4-5-8-6/h3-5H2,1-2H3
InchiKey: HTKIVHYYNMKZDN-UHFFFAOYSA-N
Formula: C6H12S2
SMILES: CCC1(C)SCCS1
Mol. weight [g/mol]: 148.29
CAS: 6008-81-7

Physical Properties

Property code	Value	Unit	Source
gf	110.42	kJ/mol	Joback Method
hf	-0.93	kJ/mol	Joback Method
hfus	6.25	kJ/mol	Joback Method
hvap	39.68	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.593		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	4000.70	kPa	Joback Method
rinpol	1136.00		NIST Webbook
rinpol	1136.00		NIST Webbook
tb	447.86	K	Joback Method
tc	688.14	K	Joback Method
tf	359.08	K	Joback Method
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.95	J/mol×K	447.86	Joback Method
cpg	241.50	J/mol×K	487.91	Joback Method
cpg	254.80	J/mol×K	527.95	Joback Method
cpg	267.00	J/mol×K	568.00	Joback Method
cpg	278.26	J/mol×K	608.04	Joback Method

cpg	288.74	J/mol×K	648.09	Joback Method
cpg	298.60	J/mol×K	688.14	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=C6008817&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