2,2-Diethyl-1,3-dithiolane

Inchi: InChI=1S/C7H14S2/c1-3-7(4-2)8-5-6-9-7/h3-6H2,1-2H3
InchiKey: FMCABCBXHDYTHA-UHFFFAOYSA-N
Formula: C7H14S2
SMILES: CCC1(CC)SCCS1
Mol. weight [g/mol]: 162.32
CAS: 26733-25-5

Physical Properties

Property code	Value	Unit	Source
gf	118.84	kJ/mol	Joback Method
hf	-21.57	kJ/mol	Joback Method
hfus	8.84	kJ/mol	Joback Method
hvap	41.91	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.983		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	3555.77	kPa	Joback Method
rinpol	1253.00		NIST Webbook
rinpol	1253.00		NIST Webbook
tb	470.74	K	Joback Method
tc	706.95	K	Joback Method
tf	370.35	K	Joback Method
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.43	J/mol×K	470.74	Joback Method
cpg	283.99	J/mol×K	510.11	Joback Method
cpg	298.32	J/mol×K	549.48	Joback Method
cpg	311.56	J/mol×K	588.85	Joback Method
cpg	323.88	J/mol×K	628.21	Joback Method
cpg	335.41	J/mol×K	667.58	Joback Method
cpg	346.34	J/mol×K	706.95	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=C26733255&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