2-Isopropyl-1,3-dithiolane

Inchi: InChI=1S/C6H12S2/c1-5(2)6-7-3-4-8-6/h5-6H,3-4H2,1-2H3
InchiKey: CMOLCULWXQDIMM-UHFFFAOYSA-N
Formula: C6H12S2
SMILES: CC(C)C1SCCS1
Mol. weight [g/mol]: 148.29
CAS: 26733-24-4

Physical Properties

Property code	Value	Unit	Source
gf	113.47	kJ/mol	Joback Method
hf	-21.45	kJ/mol	Joback Method
hfus	9.02	kJ/mol	Joback Method
hvap	40.44	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	2.449		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	3819.82	kPa	Joback Method
rinpol	1196.00		NIST Webbook
rinpol	1175.00		NIST Webbook
rinpol	1163.00		NIST Webbook
rinpol	1216.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1199.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1163.00		NIST Webbook
tb	447.18	K	Joback Method
tc	682.42	K	Joback Method
tf	320.18	K	Joback Method
vc	0.399	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.28	J/mol×K	447.18	Joback Method

cpg	241.07	J/mol×K	486.39	Joback Method
cpg	254.94	J/mol×K	525.59	Joback Method
cpg	267.93	J/mol×K	564.80	Joback Method
cpg	280.08	J/mol×K	604.01	Joback Method
cpg	291.44	J/mol×K	643.22	Joback Method
cpg	302.04	J/mol×K	682.42	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=C26733244&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