2-Isobutyl-1,3-dithiolane

Inchi: InChI=1S/C7H14S2/c1-6(2)5-7-8-3-4-9-7/h6-7H,3-5H2,1-2H3
InchiKey: BZZWMYQPYPQYLG-UHFFFAOYSA-N
Formula: C7H14S2
SMILES: CC(C)CC1SCCS1
Mol. weight [g/mol]: 162.32

Physical Properties

Property code	Value	Unit	Source
gf	121.89	kJ/mol	Joback Method
hf	-42.09	kJ/mol	Joback Method
hfus	11.61	kJ/mol	Joback Method
hvap	42.67	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.839		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
rinpol	1243.00		NIST Webbook
rinpol	1235.00		NIST Webbook
rinpol	1303.00		NIST Webbook
rinpol	1289.00		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1280.00		NIST Webbook
tb	470.06	K	Joback Method
tc	701.46	K	Joback Method
tf	331.45	K	Joback Method
vc	0.455	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.99	J/mol×K	470.06	Joback Method
cpg	283.95	J/mol×K	508.63	Joback Method
cpg	298.94	J/mol×K	547.19	Joback Method
cpg	312.99	J/mol×K	585.76	Joback Method

cpg	326.16	J/mol×K	624.33	Joback Method
cpg	338.48	J/mol×K	662.89	Joback Method
cpg	350.00	J/mol×K	701.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R78844&Units=SI
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

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