

2-Butyl-1,3-dithiolane

Inchi:	InChI=1S/C7H14S2/c1-2-3-4-7-8-5-6-9-7/h7H,2-6H2,1H3
InchiKey:	ONMLWOHLHPFOPY-UHFFFAOYSA-N
Formula:	C7H14S2
SMILES:	CCCCC1SCCS1
Mol. weight [g/mol]:	162.32

Physical Properties

Property code	Value	Unit	Source
gf	124.33	kJ/mol	Joback Method
hf	-36.81	kJ/mol	Joback Method
hfus	15.13	kJ/mol	Joback Method
hvap	43.06	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.983		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	3372.36	kPa	Joback Method
rinpol	1288.00		NIST Webbook
rinpol	1336.00		NIST Webbook
rinpol	1344.00		NIST Webbook
rinpol	1282.00		NIST Webbook
rinpol	1323.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1288.00		NIST Webbook
rinpol	1288.00		NIST Webbook
rinpol	1282.00		NIST Webbook
tb	470.50	K	Joback Method
tc	696.36	K	Joback Method
tf	346.45	K	Joback Method
vc	0.461	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.83	J/molxK	470.50	Joback Method

cpg	283.32	J/mol×K	508.14	Joback Method
cpg	297.90	J/mol×K	545.79	Joback Method
cpg	311.59	J/mol×K	583.43	Joback Method
cpg	324.44	J/mol×K	621.07	Joback Method
cpg	336.50	J/mol×K	658.72	Joback Method
cpg	347.80	J/mol×K	696.36	Joback Method

Sources

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=R78787&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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