2-Butyl-4-methyl-1,3-dithiolane

Inchi: InChI=1S/C8H16S2/c1-3-4-5-8-9-6-7(2)10-8/h7-8H,3-6H2,1-2H3
InchiKey: IHIDAFFUACTHDJ-UHFFFAOYSA-N
Formula: C8H16S2
SMILES: CCCCC1SCC(C)S1
Mol. weight [g/mol]: 176.34

Physical Properties

Property code	Value	Unit	Source
gf	125.04	kJ/mol	Joback Method
hf	-77.79	kJ/mol	Joback Method
hfus	18.80	kJ/mol	Joback Method
hvap	44.97	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.371		Crippen Method
mcvol	145.420	ml/mol	McGowan Method
pc	2918.68	kPa	Joback Method
rinpol	1320.00		NIST Webbook
rinpol	1324.00		NIST Webbook
rinpol	1368.00		NIST Webbook
rinpol	1361.00		NIST Webbook
rinpol	1320.00		NIST Webbook
rinpol	1324.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1332.00		NIST Webbook
rinpol	1324.00		NIST Webbook
tb	488.71	K	Joback Method
tc	710.71	K	Joback Method
tf	353.48	K	Joback Method
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.30	J/mol×K	488.71	Joback Method

cpg	329.20	J/mol×K	525.71	Joback Method
cpg	345.16	J/mol×K	562.71	Joback Method
cpg	360.21	J/mol×K	599.71	Joback Method
cpg	374.40	J/mol×K	636.71	Joback Method
cpg	387.75	J/mol×K	673.71	Joback Method
cpg	400.30	J/mol×K	710.71	Joback Method

Sources

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=R78808&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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