2-Butanol, 2-methyl, 3,4-bis-(methylthio)

Inchi: InChI=1S/C8H18OS2/c1-8(2,9)5-7(11-4)6-10-3/h7,9H,5-6H2,1-4H3
InchiKey: RCBRDIFTKBOJEU-UHFFFAOYSA-N
Formula: C8H18OS2
SMILES: CSCC(CC(C)(C)O)SC
Mol. weight [g/mol]: 194.36

Physical Properties

Property code	Value	Unit	Source
gf	-53.70	kJ/mol	Joback Method
hf	-290.97	kJ/mol	Joback Method
hfus	17.89	kJ/mol	Joback Method
hvap	62.03	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	2.242		Crippen Method
mcvol	162.150	ml/mol	McGowan Method
pc	2976.29	kPa	Joback Method
rinpol	1393.00		NIST Webbook
tb	608.51	K	Joback Method
tc	816.40	K	Joback Method
tf	296.96	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.95	J/mol×K	608.51	Joback Method
cpg	411.98	J/mol×K	643.16	Joback Method
cpg	424.24	J/mol×K	677.81	Joback Method
cpg	435.75	J/mol×K	712.46	Joback Method
cpg	446.53	J/mol×K	747.10	Joback Method
cpg	456.62	J/mol×K	781.75	Joback Method
cpg	466.04	J/mol×K	816.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R121618&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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