(Z)-1-(But-1-en-1-yl)-2-(sec-butyl)disulfane

Inchi: InChI=1S/C8H16S2/c1-4-6-7-9-10-8(3)5-2/h6-8H,4-5H2,1-3H3/b7-6-
InchiKey: FRHITHLONVCSDB-SREVYHEPSA-N
Formula: C8H16S2
SMILES: CCC=CSSC(C)CC
Mol. weight [g/mol]: 176.34
CAS: 110690-21-6

Physical Properties

Property code	Value	Unit	Source
gf	160.50	kJ/mol	Joback Method
hf	-12.77	kJ/mol	Joback Method
hfus	21.42	kJ/mol	Joback Method
hvap	46.61	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	4.090		Crippen Method
mcvol	151.980	ml/mol	McGowan Method
pc	2793.56	kPa	Joback Method
rinpol	1255.40		NIST Webbook
rinpol	1255.40		NIST Webbook
tb	523.72	K	Joback Method
tc	744.30	K	Joback Method
tf	228.64	K	Joback Method
vc	0.566	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.91	J/mol×K	523.72	Joback Method
cpg	337.33	J/mol×K	560.48	Joback Method
cpg	350.96	J/mol×K	597.25	Joback Method
cpg	363.82	J/mol×K	634.01	Joback Method
cpg	375.95	J/mol×K	670.77	Joback Method
cpg	387.36	J/mol×K	707.54	Joback Method
cpg	398.07	J/mol×K	744.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C110690216&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