Butane, 1-(ethenylthio)-

Other names: 3-Thia-1-heptene
Butyl vinyl sulfide
Inchi: InChI=1S/C6H12S/c1-3-5-6-7-4-2/h4H,2-3,5-6H2,1H3
InchiKey: LBMGSGLAWRZARD-UHFFFAOYSA-N
Formula: C6H12S
SMILES: C=CSCCCC
Mol. weight [g/mol]: 116.22
CAS: 4789-70-2

Physical Properties

Property code	Value	Unit	Source
gf	120.60	kJ/mol	Joback Method
hf	0.13	kJ/mol	Joback Method
hfus	14.15	kJ/mol	Joback Method
hvap	35.10	kJ/mol	Joback Method
ie	8.15 ± 0.01	eV	NIST Webbook
log10ws	-2.57		Crippen Method
logp	2.663		Crippen Method
mcvol	107.450	ml/mol	McGowan Method
pc	3322.01	kPa	Joback Method
rinpol	893.00		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	893.00		NIST Webbook
rinpol	893.00		NIST Webbook
tb	402.14	K	Joback Method
tc	595.12	K	Joback Method
tf	190.02	K	Joback Method
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.61	J/mol×K	402.14	Joback Method

cpg	202.42	J/mol×K	434.30	Joback Method
cpg	212.76	J/mol×K	466.47	Joback Method
cpg	222.66	J/mol×K	498.63	Joback Method
cpg	232.13	J/mol×K	530.79	Joback Method
cpg	241.16	J/mol×K	562.96	Joback Method
cpg	249.79	J/mol×K	595.12	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=C4789702&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
ie:	Ionization energy
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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