trans-1-(Ethylthio)-2-butene

Inchi: InChI=1S/C6H12S/c1-3-5-6-7-4-2/h3,5H,4,6H2,1-2H3/b5-3+
InchiKey: BHFZHOGCQAPTLZ-HWKANZROSA-N
Formula: C6H12S
SMILES: CC=CCSCC
Mol. weight [g/mol]: 116.22
CAS: 113664-29-2

Physical Properties

Property code	Value	Unit	Source
gf	112.98	kJ/mol	Joback Method
hf	-8.08	kJ/mol	Joback Method
hfus	15.63	kJ/mol	Joback Method
hvap	35.73	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	2.316		Crippen Method
mcvol	107.450	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
tb	409.62	K	Joback Method
tc	608.36	K	Joback Method
tf	186.70	K	Joback Method
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.21	J/mol×K	409.62	Joback Method
cpg	202.37	J/mol×K	442.74	Joback Method
cpg	213.00	J/mol×K	475.87	Joback Method
cpg	223.11	J/mol×K	508.99	Joback Method
cpg	232.74	J/mol×K	542.11	Joback Method
cpg	241.89	J/mol×K	575.24	Joback Method
cpg	250.59	J/mol×K	608.36	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C113664292&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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