2-(Ethylthio)-3-methyl-1-butene

Inchi: InChI=1S/C7H14S/c1-5-8-7(4)6(2)3/h6H,4-5H2,1-3H3
InchiKey: PWOZNERNVFOHSN-UHFFFAOYSA-N
Formula: C7H14S
SMILES: C=C(SCC)C(C)C
Mol. weight [g/mol]: 130.25
CAS: 114232-59-6

Physical Properties

Property code	Value	Unit	Source
gf	118.03	kJ/mol	Joback Method
hf	-35.58	kJ/mol	Joback Method
hfus	11.90	kJ/mol	Joback Method
hvap	37.02	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.909		Crippen Method
mcvol	121.540	ml/mol	McGowan Method
pc	3025.61	kPa	Joback Method
tb	424.46	K	Joback Method
tc	624.29	K	Joback Method
tf	172.33	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.90	J/mol×K	424.46	Joback Method
cpg	242.60	J/mol×K	457.77	Joback Method
cpg	254.73	J/mol×K	491.07	Joback Method
cpg	266.30	J/mol×K	524.38	Joback Method
cpg	277.33	J/mol×K	557.68	Joback Method
cpg	287.82	J/mol×K	590.99	Joback Method
cpg	297.80	J/mol×K	624.29	Joback Method

Sources

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=C114232596&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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