Propane, 1-(ethylthio)-2-methyl-

Other names: Sulfide, ethyl isobutyl
Ethyl isobutyl sulfide
(2-Methylpropyl) ethyl sulfide
Inchi: InChI=1S/C6H14S/c1-4-7-5-6(2)3/h6H,4-5H2,1-3H3
InchiKey: OIRKGXWQBSPXLQ-UHFFFAOYSA-N
Formula: C6H14S
SMILES: CCSCC(C)C
Mol. weight [g/mol]: 118.24
CAS: 1613-45-2

Physical Properties

Property code	Value	Unit	Source
gf	30.32	kJ/mol	Joback Method
hf	-130.58	kJ/mol	Joback Method
hfus	11.90	kJ/mol	Joback Method
hvap	35.38	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	2.396		Crippen Method
mcvol	111.750	ml/mol	McGowan Method
pc	3195.54	kPa	Joback Method
rinpol	854.00		NIST Webbook
rinpol	848.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	842.00		NIST Webbook
tb	407.40 ± 0.40	K	NIST Webbook
tc	598.38	K	Joback Method
tf	176.78	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	251.08	J/mol×K	533.93	Joback Method
cpg	261.10	J/mol×K	566.16	Joback Method
cpg	206.46	J/mol×K	405.02	Joback Method
cpg	218.30	J/mol×K	437.25	Joback Method
cpg	229.68	J/mol×K	469.47	Joback Method
cpg	240.61	J/mol×K	501.70	Joback Method
cpg	270.69	J/mol×K	598.38	Joback Method
hvapt	41.30	kJ/mol	353.00	NIST Webbook
hvapt	39.20	kJ/mol	379.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1613452&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
hvapt: Enthalpy of vaporization at a given temperature
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