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

Other names:	Sulfide, isobutyl propyl
	Isobutyl propyl sulfide
	2-Methyl-4-thiaheptane
	(2-methylpropyl) propyl sulfide
	Propyl 2-methylpropylsulfide
	Propyl isobutyl sulfide
Inchi:	InChI=1S/C7H16S/c1-4-5-8-6-7(2)3/h7H,4-6H2,1-3H3
InchiKey:	YZCUJPLKGSDCFP-UHFFFAOYSA-N
Formula:	C7H16S
SMILES:	CCCSCC(C)C
Mol. weight [g/mol]:	132.27
CAS:	1741-84-0

Physical Properties

Property code	Value	Unit	Source
gf	38.74	kJ/mol	Joback Method
hf	-151.22	kJ/mol	Joback Method
hfus	14.49	kJ/mol	Joback Method
hvap	37.61	kJ/mol	Joback Method
ie	8.40 ± 0.05	eV	NIST Webbook
log10ws	-2.39		Crippen Method
logp	2.786		Crippen Method
mcvol	125.840	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
rinpol	941.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	936.00		NIST Webbook
tb	427.90	K	Joback Method
tc	619.57	K	Joback Method
tf	188.05	K	Joback Method
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.63	J/mol×K	427.90	Joback Method
cpg	258.76	J/mol×K	459.85	Joback Method
cpg	271.36	J/mol×K	491.79	Joback Method
cpg	283.45	J/mol×K	523.74	Joback Method
cpg	295.02	J/mol×K	555.68	Joback Method
cpg	306.08	J/mol×K	587.63	Joback Method
cpg	316.66	J/mol×K	619.57	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1741840&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
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