3-methyl-4-thiaheptane

Other names:	Propyl 2-butyl sulfide
	Propyl (1-methylpropyl) sulfide
	(1-methylpropyl) propyl sulfide
	Sulfide, propyl 1-methylpropyl
Inchi:	InChI=1S/C7H16S/c1-4-6-8-7(3)5-2/h7H,4-6H2,1-3H3
InchiKey:	ZGVPENKHDNEGTK-UHFFFAOYSA-N
Formula:	C7H16S
SMILES:	CCCSC(C)CC
Mol. weight [g/mol]:	132.27

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
log10ws	-2.75		Crippen Method
logp	2.928		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	946.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	940.00		NIST Webbook
rinpol	951.00		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

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=R5166&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume