6-methyl-3-thiaheptane

Other names: (3-methylbutyl) ethyl sulfide
Inchi: InChI=1S/C7H16S/c1-4-8-6-5-7(2)3/h7H,4-6H2,1-3H3
InchiKey: AGKOQHSTPVLJSQ-UHFFFAOYSA-N
Formula: C7H16S
SMILES: CCSCCC(C)C
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	-2.39		Crippen Method
logp	2.786		Crippen Method
mcvol	125.840	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
rinpol	954.00		NIST Webbook
rinpol	954.00		NIST Webbook
rinpol	954.00		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=R157578&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