Heptane, 1,1'-thiobis-

Other names:	Heptyl sulfide
	Diheptyl sulfide
	n-Heptyl sulfide
	di-n-Heptyl sulfide
	diheptyl sulphide
Inchi:	InChI=1S/C14H30S/c1-3-5-7-9-11-13-15-14-12-10-8-6-4-2/h3-14H2,1-2H3
InchiKey:	LEMIDOZYVQXGLI-UHFFFAOYSA-N
Formula:	C14H30S
SMILES:	CCCCCCCSCCCCCCC
Mol. weight [g/mol]:	230.45
CAS:	629-65-2

Physical Properties

Property code	Value	Unit	Source
gf	100.12	kJ/mol	Joback Method
hf	-290.42	kJ/mol	Joback Method
hfus	36.15	kJ/mol	Joback Method
hvap	53.58	kJ/mol	Joback Method
log10ws	-5.57		Crippen Method
logp	5.660		Crippen Method
mcvol	224.470	ml/mol	McGowan Method
pc	1543.92	kPa	Joback Method
rinpol	1674.00		NIST Webbook
rinpol	1696.00		NIST Webbook
rinpol	1682.00		NIST Webbook
rinpol	1674.00		NIST Webbook
tb	588.50	K	Joback Method
tc	763.97	K	Joback Method
tf	281.94	K	Joback Method
vc	0.874	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	575.87	J/mol×K	588.50	Joback Method
cpg	594.19	J/mol×K	617.74	Joback Method
cpg	611.71	J/mol×K	646.99	Joback Method
cpg	628.47	J/mol×K	676.23	Joback Method
cpg	644.48	J/mol×K	705.48	Joback Method
cpg	659.75	J/mol×K	734.72	Joback Method
cpg	674.32	J/mol×K	763.97	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C629652&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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