Propane, 1,1'-thiobis[3-chloro-

Other names: Bis(3-chloropropyl) sulfide
Inchi: InChI=1S/C6H12Cl2S/c7-3-1-5-9-6-2-4-8/h1-6H2
InchiKey: VDTHWBLOSZIMMN-UHFFFAOYSA-N
Formula: C6H12Cl2S
SMILES: ClCCCSCCCCl
Mol. weight [g/mol]: 187.13
CAS: 55882-21-8

Physical Properties

Property code	Value	Unit	Source
gf	8.90	kJ/mol	Joback Method
hf	-156.78	kJ/mol	Joback Method
hfus	23.82	kJ/mol	Joback Method
hvap	44.54	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.977		Crippen Method
mcvol	136.230	ml/mol	McGowan Method
pc	2918.68	kPa	Joback Method
rinpol	1275.60		NIST Webbook
rinpol	1236.00		NIST Webbook
rinpol	1311.00		NIST Webbook
rinpol	1236.00		NIST Webbook
rinpol	1275.60		NIST Webbook
rinpol	1236.00		NIST Webbook
tb	480.32	K	Joback Method
tc	682.49	K	Joback Method
tf	251.62	K	Joback Method
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.92	J/mol×K	480.32	Joback Method
cpg	268.63	J/mol×K	514.02	Joback Method

cpg	278.83	J/mol×K	547.71	Joback Method
cpg	288.52	J/mol×K	581.41	Joback Method
cpg	297.74	J/mol×K	615.10	Joback Method
cpg	306.47	J/mol×K	648.80	Joback Method
cpg	314.74	J/mol×K	682.49	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55882218&Units=SI

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