2,4,6,8,9,10-Hexathiatricyclo[3.3.1.1(3,7)]decane, 1,3,5,7-tetramethyl-

Other names:	2,4,6,8,9,10-Hexathiaadamantane, 1,3,5,7-tetramethyl-
	Tetramethylhexathiaadamantane
	1,3,5,7-Tetramethyl-2,4,6,8,9,10-hexathiaadamantane
	1,3,5,7-Tetramethyl-2,4,6,8,9,10-hexathioadamantane
Inchi:	InChI=1S/C8H12S6/c1-5-9-6(2)12-7(3,10-5)14-8(4,11-5)13-6/h1-4H3
InchiKey:	APZGKGHAXUURNO-UHFFFAOYSA-N
Formula:	C8H12S6
SMILES:	CC12SC3(C)SC(C)(S1)SC(C)(S2)S3
Mol. weight [g/mol]:	300.57
CAS:	6327-74-8

Physical Properties

Property code	Value	Unit	Source
gf	396.12	kJ/mol	Joback Method
hf	315.97	kJ/mol	Joback Method
hfus	6.60	kJ/mol	Joback Method
hvap	63.27	kJ/mol	Joback Method
log10ws	-6.57		Crippen Method
logp	5.121		Crippen Method
mcvol	189.100	ml/mol	McGowan Method
pc	4691.31	kPa	Joback Method
ss	321.12	J/mol×K	NIST Webbook
tb	690.20	K	Joback Method
tc	1048.17	K	Joback Method
tf	822.28	K	Joback Method
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.15	J/mol×K	928.85	Joback Method
cpg	558.99	J/mol×K	988.51	Joback Method
cpg	442.24	J/mol×K	690.20	Joback Method
cpg	457.09	J/mol×K	749.86	Joback Method

cpg	474.20	J/mol×K	809.52	Joback Method
cpg	495.55	J/mol×K	869.18	Joback Method
cpg	605.08	J/mol×K	1048.17	Joback Method
cps	301.62	J/mol×K	298.15	NIST Webbook
hfust	23.70	kJ/mol	501.40	NIST Webbook

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=C6327748&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
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume