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

Other names: 2,4,6,8-Tetrathiaadamantane, 1,3,5,7-tetramethyl-
Tetramethyltetrathiaadamantane
1,3,5,7-Tetramethyl-2,4,6,8-tetrathiaadamantane
2,4,6,8-Tetrathiatricyclo[3.3.1.13,7]decane, 1,3,5,7-tetramethyl-

Inchi: InChI=1S/C10H16S4/c1-7-5-8(2)13-9(3,11-7)6-10(4,12-7)14-8/h5-6H2,1-4H3

InchiKey: HUWTULKGEASRFA-UHFFFAOYSA-N

Formula: C10H16S4

SMILES: CC12CC3(C)SC(C)(CC(C)(S1)S3)S2

Mol. weight [g/mol]: 264.49

CAS: 7000-79-5

Physical Properties

Property code	Value	Unit	Source
chs	-8477.00 ± 3.00	kJ/mol	NIST Webbook
gf	333.24	kJ/mol	Joback Method
hf	-37.00 ± 5.00	kJ/mol	NIST Webbook
hfs	-154.00 ± 3.00	kJ/mol	NIST Webbook
hfus	4.47	kJ/mol	Joback Method
hsub	117.00	kJ/mol	NIST Webbook
hsub	117.10 ± 4.10	kJ/mol	NIST Webbook
hsub	117.00 ± 4.20	kJ/mol	NIST Webbook
hvap	56.10	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	4.605		Crippen Method
mcvol	184.580	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
ss	300.83	J/mol×K	NIST Webbook
tb	640.30	K	Joback Method
tc	954.09	K	Joback Method
tf	677.92	K	Joback Method
vc	0.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.18	J/mol×K	640.30	Joback Method
cpg	476.80	J/mol×K	692.60	Joback Method
cpg	493.34	J/mol×K	744.90	Joback Method
cpg	511.18	J/mol×K	797.19	Joback Method
cpg	531.65	J/mol×K	849.49	Joback Method
cpg	556.10	J/mol×K	901.79	Joback Method
cpg	585.90	J/mol×K	954.09	Joback Method
cps	295.85	J/mol×K	298.15	NIST Webbook

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=C7000795&Units=SI

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
cps: Solid phase heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsub: Enthalpy of sublimation 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
ss: Solid phase molar entropy at standard conditions
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume