

7-Thiabicyclo[2.2.1]heptane

Other names:	7-Thianorboranane
Inchi:	InChI=1S/C6H10S/c1-2-6-4-3-5(1)7-6/h5-6H,1-4H2
InchiKey:	YADULIHSBVCGOJ-UHFFFAOYSA-N
Formula:	C6H10S
SMILES:	C1CC2CCC1S2
Mol. weight [g/mol]:	114.21
CAS:	279-59-4

Physical Properties

Property code	Value	Unit	Source
gf	148.90	kJ/mol	Joback Method
hf	17.53	kJ/mol	Joback Method
hfus	9.12	kJ/mol	Joback Method
hvap	34.76	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	2.044		Crippen Method
mcvol	90.030	ml/mol	McGowan Method
pc	4356.87	kPa	Joback Method
tb	402.26	K	Joback Method
tc	625.03	K	Joback Method
tf	273.19	K	Joback Method
vc	0.324	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	167.53	J/mol×K	402.26	Joback Method
cpg	182.56	J/mol×K	439.39	Joback Method
cpg	196.48	J/mol×K	476.52	Joback Method
cpg	209.36	J/mol×K	513.65	Joback Method
cpg	221.28	J/mol×K	550.77	Joback Method
cpg	232.32	J/mol×K	587.90	Joback Method
cpg	242.53	J/mol×K	625.03	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=C279594&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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