8-Methylene-trans-3-thiabicyclo[4.4.0]decane

Inchi: InChI=1S/C10H16S/c1-8-2-3-10-7-11-5-4-9(10)6-8/h9-10H,1-7H2/t9-,10+/m0/s1
InchiKey: WQEZQTRTRLMBTM-VHSXEESVSA-N
Formula: C10H16S
SMILES: C=C1CCC2CSCCC2C1
Mol. weight [g/mol]: 168.30
CAS: 77471-73-9

Physical Properties

Property code	Value	Unit	Source
gf	199.36	kJ/mol	Joback Method
hf	0.73	kJ/mol	Joback Method
hfus	12.02	kJ/mol	Joback Method
hvap	44.34	kJ/mol	Joback Method
ie	8.26	eV	NIST Webbook
log10ws	-3.05		Crippen Method
logp	3.096		Crippen Method
mcvol	142.090	ml/mol	McGowan Method
pc	3069.34	kPa	Joback Method
tb	505.75	K	Joback Method
tc	744.34	K	Joback Method
tf	321.39	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.56	J/mol×K	505.75	Joback Method
cpg	343.04	J/mol×K	545.51	Joback Method
cpg	362.16	J/mol×K	585.28	Joback Method
cpg	379.98	J/mol×K	625.04	Joback Method
cpg	396.58	J/mol×K	664.81	Joback Method
cpg	412.01	J/mol×K	704.57	Joback Method
cpg	426.33	J/mol×K	744.34	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=C77471739&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
ie:	Ionization energy
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