4-methyl-2-thiaadamantane

Inchi: InChI=1S/C10H16S/c1-6-8-2-7-3-9(5-8)11-10(6)4-7/h6-10H,2-5H2,1H3
InchiKey: ZBBUECPKKSCLQX-UHFFFAOYSA-N
Formula: C10H16S
SMILES: CC1C2CC3CC(C2)SC1C3
Mol. weight [g/mol]: 168.30

Physical Properties

Property code	Value	Unit	Source
gf	227.91	kJ/mol	Joback Method
hf	-32.91	kJ/mol	Joback Method
hfus	19.76	kJ/mol	Joback Method
hvap	42.96	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.926		Crippen Method
mcvol	135.530	ml/mol	McGowan Method
pc	2969.80	kPa	Joback Method
rinpol	1505.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1531.00		NIST Webbook
rinpol	1517.00		NIST Webbook
rinpol	1505.00		NIST Webbook
rinpol	1518.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1531.00		NIST Webbook
tb	491.18	K	Joback Method
tc	718.92	K	Joback Method
tf	327.73	K	Joback Method
vc	0.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.26	J/mol×K	491.18	Joback Method
cpg	347.19	J/mol×K	529.14	Joback Method

cpg	366.61	J/mol×K	567.09	Joback Method
cpg	384.63	J/mol×K	605.05	Joback Method
cpg	401.37	J/mol×K	643.01	Joback Method
cpg	416.93	J/mol×K	680.97	Joback Method
cpg	431.42	J/mol×K	718.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R138780&Units=SI
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

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