Bicyclo[2.2.1]heptane-2-thione, 1,7,7-trimethyl-

Other names:	2-Bornanethione
	Thiocamphor
Inchi:	InChI=1S/C10H16S/c1-9(2)7-4-5-10(9,3)8(11)6-7/h7H,4-6H2,1-3H3
InchiKey:	AAADKYXUTOBAGS-UHFFFAOYSA-N
Formula:	C10H16S
SMILES:	CC12CCC(CC1=S)C2(C)C
Mol. weight [g/mol]:	168.30
CAS:	7519-74-6

Physical Properties

Property code	Value	Unit	Source
affp	883.90	kJ/mol	NIST Webbook
basg	852.00	kJ/mol	NIST Webbook
gf	214.88	kJ/mol	Joback Method
hf	14.95	kJ/mol	Joback Method
hfus	10.33	kJ/mol	Joback Method
hvap	42.72	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	3.203		Crippen Method
mcvol	142.090	ml/mol	McGowan Method
pc	3184.73	kPa	Joback Method
tb	514.40	K	Joback Method
tc	751.23	K	Joback Method
tf	342.05	K	Joback Method
vc	0.534	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.24	J/mol×K	514.40	Joback Method
cpg	350.23	J/mol×K	553.87	Joback Method
cpg	365.61	J/mol×K	593.34	Joback Method
cpg	379.71	J/mol×K	632.81	Joback Method
cpg	392.86	J/mol×K	672.28	Joback Method

cpg	405.40	J/mol×K	711.76	Joback Method
cpg	417.65	J/mol×K	751.23	Joback Method

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=C7519746&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
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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