4,7,7-Trimethyl-6-thiabicyclo[3.2.1]octane

Other names: 2,8-Epithio-cis-p-menthane
Inchi: InChI=1S/C10H18S/c1-7-4-5-8-6-9(7)11-10(8,2)3/h7-9H,4-6H2,1-3H3
InchiKey: FAXNZPOZWCWYBD-UHFFFAOYSA-N
Formula: C10H18S
SMILES: CC1CCC2CC1SC2(C)C
Mol. weight [g/mol]: 170.31

Physical Properties

Property code	Value	Unit	Source
gf	149.57	kJ/mol	Joback Method
hf	-96.63	kJ/mol	Joback Method
hfus	13.23	kJ/mol	Joback Method
hvap	42.07	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.317		Crippen Method
mcvol	146.390	ml/mol	McGowan Method
pc	2784.72	kPa	Joback Method
tb	488.95	K	Joback Method
tc	717.20	K	Joback Method
tf	330.17	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.52	J/mol×K	488.95	Joback Method
cpg	361.27	J/mol×K	526.99	Joback Method
cpg	380.51	J/mol×K	565.03	Joback Method
cpg	398.41	J/mol×K	603.07	Joback Method
cpg	415.11	J/mol×K	641.12	Joback Method
cpg	430.80	J/mol×K	679.16	Joback Method
cpg	445.63	J/mol×K	717.20	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=U306335&Units=SI

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