2H-1-Benzothiopyran, octahydro-2-methyl-

Inchi: InChI=1S/C10H18S/c1-8-6-7-9-4-2-3-5-10(9)11-8/h8-10H,2-7H2,1H3
InchiKey: UXIZJMFBZMPJGD-UHFFFAOYSA-N
Formula: C10H18S
SMILES: CC1CCC2CCCCC2S1
Mol. weight [g/mol]: 170.31
CAS: 42900-28-7

Physical Properties

Property code	Value	Unit	Source
gf	138.57	kJ/mol	Joback Method
hf	-103.85	kJ/mol	Joback Method
hfus	14.25	kJ/mol	Joback Method
hvap	43.87	kJ/mol	Joback Method
ie	7.76 ± 0.01	eV	NIST Webbook
log10ws	-3.66		Crippen Method
logp	3.461		Crippen Method
mcvol	146.390	ml/mol	McGowan Method
pc	2899.85	kPa	Joback Method
tb	501.92	K	Joback Method
tc	738.14	K	Joback Method
tf	303.47	K	Joback Method
vc	0.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.64	J/mol×K	501.92	Joback Method
cpg	363.15	J/mol×K	541.29	Joback Method
cpg	384.20	J/mol×K	580.66	Joback Method
cpg	403.88	J/mol×K	620.03	Joback Method
cpg	422.23	J/mol×K	659.40	Joback Method
cpg	439.32	J/mol×K	698.77	Joback Method
cpg	455.21	J/mol×K	738.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C42900287&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

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