7-Thiabicyclo[4.1.0]heptane

Other names:	Cyclohexane, 1,2-epithio-
	Cyclohexene episulfide
	Cyclohexene sulfide
	1,2-Cyclohexylene sulfide
	1,2-epithiocyclohexane
Inchi:	InChI=1S/C6H10S/c1-2-4-6-5(3-1)7-6/h5-6H,1-4H2
InchiKey:	PQWJNIJNYRPOAA-UHFFFAOYSA-N
Formula:	C6H10S
SMILES:	C1CCC2SC2C1
Mol. weight [g/mol]:	114.21
CAS:	286-28-2

Physical Properties

Property code	Value	Unit	Source
gf	148.90	kJ/mol	Joback Method
hf	17.53	kJ/mol	Joback Method
hfus	9.12	kJ/mol	Joback Method
hvap	34.76	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	2.044		Crippen Method
mcvol	90.030	ml/mol	McGowan Method
pc	4356.87	kPa	Joback Method
ripol	1390.00		NIST Webbook
tb	402.26	K	Joback Method
tc	625.03	K	Joback Method
tf	273.19	K	Joback Method
vc	0.324	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	167.53	J/mol×K	402.26	Joback Method
cpg	182.56	J/mol×K	439.39	Joback Method
cpg	196.48	J/mol×K	476.52	Joback Method

cpg	209.36	J/mol×K	513.65	Joback Method
cpg	221.28	J/mol×K	550.77	Joback Method
cpg	232.32	J/mol×K	587.90	Joback Method
cpg	242.53	J/mol×K	625.03	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	329.70	K	1.60	NIST Webbook

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=C286282&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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume