trans-2-Methylthiolan-3-ol

Inchi: InChI=1S/C5H10OS/c1-4-5(6)2-3-7-4/h4-6H,2-3H2,1H3/t4-,5+/m1/s1
InchiKey: HAUQWGSXLBQNPN-UHNVWZDZSA-N
Formula: C5H10OS
SMILES: CC1SCCC1O
Mol. weight [g/mol]: 118.20

Physical Properties

Property code	Value	Unit	Source
gf	-76.90	kJ/mol	Joback Method
hf	-213.36	kJ/mol	Joback Method
hfus	11.46	kJ/mol	Joback Method
hvap	49.16	kJ/mol	Joback Method
log10ws	-1.18		Crippen Method
logp	0.873		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	4659.34	kPa	Joback Method
ripol	1782.00		NIST Webbook
tb	464.42	K	Joback Method
tc	667.56	K	Joback Method
tf	297.04	K	Joback Method
vc	0.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	192.80	J/mol×K	464.42	Joback Method
cpg	204.02	J/mol×K	498.28	Joback Method
cpg	214.66	J/mol×K	532.13	Joback Method
cpg	224.73	J/mol×K	565.99	Joback Method
cpg	234.27	J/mol×K	599.84	Joback Method
cpg	243.28	J/mol×K	633.70	Joback Method
cpg	251.78	J/mol×K	667.56	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=R410918&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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