(E)-2-methyl-3-tetrahydrofuranthiol

Inchi: InChI=1S/C5H10OS/c1-4-5(7)2-3-6-4/h4-5,7H,2-3H2,1H3
InchiKey: DBPHPBLAKVZXOY-UHFFFAOYSA-N
Formula: C5H10OS
SMILES: CC1OCCC1S
Mol. weight [g/mol]: 118.20
CAS: 26548-78-7

Physical Properties

Property code	Value	Unit	Source
gf	-36.67	kJ/mol	Joback Method
hf	-199.91	kJ/mol	Joback Method
hfus	15.73	kJ/mol	Joback Method
hvap	37.92	kJ/mol	Joback Method
log10ws	-1.19		Crippen Method
logp	1.094		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	4468.24	kPa	Joback Method
ripol	1315.00		NIST Webbook
ripol	1315.00		NIST Webbook
tb	414.22	K	Joback Method
tc	639.42	K	Joback Method
tf	215.80	K	Joback Method
vc	0.331	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	175.61	J/mol×K	414.22	Joback Method
cpg	188.95	J/mol×K	451.75	Joback Method
cpg	201.58	J/mol×K	489.29	Joback Method
cpg	213.52	J/mol×K	526.82	Joback Method
cpg	224.78	J/mol×K	564.36	Joback Method
cpg	235.39	J/mol×K	601.89	Joback Method
cpg	245.36	J/mol×K	639.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26548787&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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