2-Buten-1-thiol

Inchi: InChI=1S/C4H8S/c1-2-3-4-5/h2-3,5H,4H2,1H3/b3-2+
InchiKey: PSKWBKFCLVNPMT-NSCUHMNNSA-N
Formula: C4H8S
SMILES: CC=CCS
Mol. weight [g/mol]: 88.17

Physical Properties

Property code	Value	Unit	Source
gf	92.41	kJ/mol	Joback Method
hf	29.81	kJ/mol	Joback Method
hfus	10.36	kJ/mol	Joback Method
hvap	31.19	kJ/mol	Joback Method
log10ws	-1.42		Crippen Method
logp	1.492		Crippen Method
mcvol	79.270	ml/mol	McGowan Method
pc	4528.58	kPa	Joback Method
rinpol	704.00		NIST Webbook
tb	357.94	K	Joback Method
tc	559.37	K	Joback Method
tf	166.22	K	Joback Method
vc	0.293	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	119.94	J/mol×K	357.94	Joback Method
cpg	128.13	J/mol×K	391.51	Joback Method
cpg	135.88	J/mol×K	425.08	Joback Method
cpg	143.21	J/mol×K	458.65	Joback Method
cpg	150.15	J/mol×K	492.22	Joback Method
cpg	156.70	J/mol×K	525.80	Joback Method
cpg	162.89	J/mol×K	559.37	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=R510979&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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