2-Methyl-2-butene-1-thiol

Other names: 2-Methyl-2-buten-1-thiol
2-METHYL-3-BUTENE-2-THIOL
Inchi: InChI=1S/C5H10S/c1-3-5(2)4-6/h3,6H,4H2,1-2H3
InchiKey: ZKDRFRZNMQYWPD-UHFFFAOYSA-N
Formula: C5H10S
SMILES: CC=C(C)CS
Mol. weight [g/mol]: 102.20

Physical Properties

Property code	Value	Unit	Source
af	0.3033		Cheméo Relay (1.0)
gf	92.28	kJ/mol	Joback Method
hf	-29.65	kJ/mol	Cheméo Relay (1.0)
hfus	11.64	kJ/mol	Joback Method
hvap	45.52	kJ/mol	Cheméo Relay (1.0)
ie	8.44	eV	Cheméo Relay (1.0)
logp	1.882		Crippen Method
mcvol	93.360	ml/mol	McGowan Method
pc	4021.02	kPa	Joback Method
rinpol	823.00		NIST Webbook
rinpol	823.00		NIST Webbook
tb	392.70	K	Cheméo Relay (1.0)
tc	597.41	K	Cheméo Relay (1.0)
tf	164.55	K	Cheméo Relay (1.0)
vc	0.330	m3/kmol	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-6.39000e-01
Coeff. B	5.26040e-01

Coeff. C	-3.56700e-04
Coeff. D	1.03100e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U99454&Units=SI

Legend

af:	Acentric Factor
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
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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