2-METHYL-3-BUTENE-2-THIOL

Other names: 2-Methyl-2-buten-1-thiol
Inchi: InChI=1S/C5H10S/c1-3-5(2)4-6/h3,6H,4H2,1-2H3/b5-3-
InchiKey: ZKDRFRZNMQYWPD-HWKANZROSA-N
Formula: C5H10S
SMILES: C/C=C(\C)CS
Mol. weight [g/mol]: 102.20

Physical Properties

Property code	Value	Unit	Source
af	0.2918		Cheméo Relay (1.0)
gf	92.28	kJ/mol	Joback Method
hf	-16.78	kJ/mol	Cheméo Relay (1.0)
hfus	11.64	kJ/mol	Joback Method
hvap	42.10	kJ/mol	Cheméo Relay (1.0)
ie	8.51	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	387.49	K	Cheméo Relay (1.0)
tc	594.66	K	Cheméo Relay (1.0)
tf	166.32	K	Cheméo Relay (1.0)
vc	0.332	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	153.62	J/mol×K	380.70	Joback Method
cpg	163.54	J/mol×K	414.78	Joback Method
cpg	172.94	J/mol×K	448.85	Joback Method
cpg	181.82	J/mol×K	482.93	Joback Method
cpg	190.23	J/mol×K	517.01	Joback Method
cpg	198.18	J/mol×K	551.09	Joback Method

cpg	205.70	J/mol×K	585.16	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U99454&Units=SI

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):

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