

3-Methylpentan-2-thiol, threo

Inchi:	InChI=1S/C6H14S/c1-4-5(2)6(3)7/h5-7H,4H2,1-3H3/t5-,6+/m0/s1
InchiKey:	KKRNXWOGSCUFIT-NTSWFWBYSA-N
Formula:	C6H14S
SMILES:	CCC(C)C(C)S
Mol. weight [g/mol]:	118.24

Physical Properties

Property code	Value	Unit	Source
gf	24.15	kJ/mol	Joback Method
hf	-139.25	kJ/mol	Joback Method
hfus	8.29	kJ/mol	Joback Method
hvap	34.91	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.351		Crippen Method
mcvol	111.750	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
rinpol	847.00		NIST Webbook
rinpol	847.00		NIST Webbook
tb	398.66	K	Joback Method
tc	596.55	K	Joback Method
tf	163.84	K	Joback Method
vc	0.413	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.76	J/mol×K	398.66	Joback Method
cpg	217.01	J/mol×K	431.64	Joback Method
cpg	228.72	J/mol×K	464.62	Joback Method
cpg	239.90	J/mol×K	497.61	Joback Method
cpg	250.57	J/mol×K	530.59	Joback Method
cpg	260.75	J/mol×K	563.57	Joback Method
cpg	270.44	J/mol×K	596.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R524280&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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