

4-Mercapto-3-methylpentan-2-one

Inchi: InChI=1S/C6H12OS/c1-4(5(2)7)6(3)8/h4,6,8H,1-3H3
InchiKey: VPFDUTYZTDYOAS-UHFFFAOYSA-N
Formula: C6H12OS
SMILES: CC(=O)C(C)C(C)S
Mol. weight [g/mol]: 132.22

Physical Properties

Property code	Value	Unit	Source
gf	-104.77	kJ/mol	Joback Method
hf	-251.83	kJ/mol	Joback Method
hfus	9.89	kJ/mol	Joback Method
hvap	41.66	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	1.530		Crippen Method
mcvol	113.320	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
rinpol	959.00		NIST Webbook
rinpol	967.00		NIST Webbook
rinpol	967.00		NIST Webbook
rinpol	1002.00		NIST Webbook
rinpol	967.00		NIST Webbook
rinpol	959.00		NIST Webbook
rinpol	959.00		NIST Webbook
rinpol	967.00		NIST Webbook
rinpol	994.00		NIST Webbook
rinpol	967.00		NIST Webbook
rinpol	1002.00		NIST Webbook
ripol	1469.00		NIST Webbook
ripol	1477.00		NIST Webbook
ripol	1469.00		NIST Webbook
tb	452.53	K	Joback Method
tc	662.92	K	Joback Method
tf	213.77	K	Joback Method
vc	0.419	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.16	J/mol×K	452.53	Joback Method
cpg	233.66	J/mol×K	487.60	Joback Method
cpg	244.60	J/mol×K	522.66	Joback Method
cpg	254.97	J/mol×K	557.73	Joback Method
cpg	264.81	J/mol×K	592.79	Joback Method
cpg	274.12	J/mol×K	627.86	Joback Method
cpg	282.93	J/mol×K	662.92	Joback Method

Sources

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=R205499&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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