

4-mercapto-4-methyl-2-pentanol

Other names:	4-mercapto-4-methyl pentan-2-ol 4-methyl-4-mercapto-2-pentanol 2-Pentanol, 4-mercapto-4-methyl
Inchi:	InChI=1S/C6H14OS/c1-5(7)4-6(2,3)8/h5,7-8H,4H2,1-3H3
InchiKey:	FDBQLLMYSACL PB-UHFFFAOYSA-N
Formula:	C6H14OS
SMILES:	CC(O)CC(C)(C)S
Mol. weight [g/mol]:	134.24
CAS:	255391-65-2

Physical Properties

Property code	Value	Unit	Source
gf	-107.39	kJ/mol	Joback Method
hf	-294.95	kJ/mol	Joback Method
hfus	8.49	kJ/mol	Joback Method
hvap	50.68	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.466		Crippen Method
mcvol	117.620	ml/mol	McGowan Method
pc	3853.09	kPa	Joback Method
ripol	976.00		NIST Webbook
ripol	1042.00		NIST Webbook
ripol	976.00		NIST Webbook
ripol	1042.00		NIST Webbook
ripol	1042.00		NIST Webbook
ripol	1039.00		NIST Webbook
ripol	1039.00		NIST Webbook
ripol	1567.00		NIST Webbook
ripol	1567.00		NIST Webbook
ripol	1534.00		NIST Webbook
ripol	1547.00		NIST Webbook
ripol	1547.00		NIST Webbook
ripol	1534.00		NIST Webbook
tb	488.05	K	Joback Method
tc	683.77	K	Joback Method
tf	242.08	K	Joback Method
vc	0.427	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.48	J/mol×K	488.05	Joback Method
cpg	267.70	J/mol×K	520.67	Joback Method
cpg	278.28	J/mol×K	553.29	Joback Method
cpg	288.26	J/mol×K	585.91	Joback Method
cpg	297.65	J/mol×K	618.53	Joback Method
cpg	306.50	J/mol×K	651.15	Joback Method
cpg	314.83	J/mol×K	683.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C255391652&Units=SI
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

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
rinol:	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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