4-Mercapto-3-methyl-2-pentanone, # 2

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	967.00		NIST Webbook
rinpol	967.00		NIST Webbook
tb	452.53	K	Joback Method
tc	662.92	K	Joback Method
tf	213.77	K	Joback Method
vc	0.419	m3/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=R603031&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume