3-mercapto-2-butanone

Other names: 2-Butanone, 3-mercapto-
3-mercaptobutan-2-one
Inchi: InChI=1S/C4H8OS/c1-3(5)4(2)6/h4,6H,1-2H3
InchiKey: XLMPYCGSRHSSSX-UHFFFAOYSA-N
Formula: C4H8OS
SMILES: CC(=O)C(C)S
Mol. weight [g/mol]: 104.17
CAS: 40789-98-8

Physical Properties

Property code	Value	Unit	Source
gf	-119.17	kJ/mol	Joback Method
hf	-205.27	kJ/mol	Joback Method
hfus	8.23	kJ/mol	Joback Method
hvap	37.59	kJ/mol	Joback Method
log10ws	-0.96		Crippen Method
logp	0.894		Crippen Method
mcvol	85.140	ml/mol	McGowan Method
pc	4646.65	kPa	Joback Method
rinpol	837.00		NIST Webbook
rinpol	817.00		NIST Webbook
rinpol	823.00		NIST Webbook
rinpol	823.00		NIST Webbook
rinpol	816.00		NIST Webbook
rinpol	817.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	815.00		NIST Webbook
rinpol	780.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	798.00		NIST Webbook
rinpol	789.00		NIST Webbook
rinpol	821.00		NIST Webbook
rinpol	787.00		NIST Webbook
rinpol	818.00		NIST Webbook
rinpol	768.00		NIST Webbook

rinpol	811.00		NIST Webbook
rinpol	816.00		NIST Webbook
rinpol	817.00		NIST Webbook
rinpol	787.00		NIST Webbook
ripol	1282.00		NIST Webbook
ripol	1295.00		NIST Webbook
ripol	1283.00		NIST Webbook
ripol	1264.00		NIST Webbook
ripol	1282.00		NIST Webbook
ripol	1282.00		NIST Webbook
ripol	1282.00		NIST Webbook
ripol	1282.00		NIST Webbook
ripol	1282.00		NIST Webbook
ripol	1283.00		NIST Webbook
ripol	1295.00		NIST Webbook
tb	407.21	K	Joback Method
tc	617.59	K	Joback Method
tf	206.23	K	Joback Method
vc	0.314	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	147.15	J/mol×K	407.21	Joback Method
cpg	155.43	J/mol×K	442.27	Joback Method
cpg	163.32	J/mol×K	477.34	Joback Method
cpg	170.84	J/mol×K	512.40	Joback Method
cpg	177.98	J/mol×K	547.46	Joback Method
cpg	184.76	J/mol×K	582.52	Joback Method
cpg	191.18	J/mol×K	617.59	Joback Method

Sources

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=C40789988&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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