1-Mercaptobutan-3-one

Inchi: InChI=1S/C4H8OS/c1-4(5)2-3-6/h6H,2-3H2,1H3
InchiKey: LBFXPJUFQGXMJY-UHFFFAOYSA-N
Formula: C4H8OS
SMILES: CC(=O)CCS
Mol. weight [g/mol]: 104.17

Physical Properties

Property code	Value	Unit	Source
gf	-116.73	kJ/mol	Joback Method
hf	-199.99	kJ/mol	Joback Method
hfus	11.76	kJ/mol	Joback Method
hvap	37.98	kJ/mol	Joback Method
log10ws	-0.85		Crippen Method
logp	0.895		Crippen Method
mcvol	85.140	ml/mol	McGowan Method
pc	4596.38	kPa	Joback Method
rinpol	844.00		NIST Webbook
rinpol	844.00		NIST Webbook
rinpol	844.00		NIST Webbook
rinpol	844.00		NIST Webbook
ripol	1445.00		NIST Webbook
ripol	1445.00		NIST Webbook
tb	407.65	K	Joback Method
tc	612.92	K	Joback Method
tf	221.23	K	Joback Method
vc	0.320	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	147.09	J/mol×K	407.65	Joback Method
cpg	155.07	J/mol×K	441.86	Joback Method
cpg	162.69	J/mol×K	476.07	Joback Method
cpg	169.95	J/mol×K	510.28	Joback Method

cpg	176.88	J/mol×K	544.50	Joback Method
cpg	183.46	J/mol×K	578.71	Joback Method
cpg	189.72	J/mol×K	612.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R291940&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
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