3-Mercaptopropylacetate

Inchi: InChI=1S/C5H10O2S/c1-5(6)7-3-2-4-8/h8H,2-4H2,1H3
InchiKey: FVSBSLZVZIYRRO-UHFFFAOYSA-N
Formula: C5H10O2S
SMILES: CC(=O)OCCCS
Mol. weight [g/mol]: 134.20

Physical Properties

Property code	Value	Unit	Source
gf	-213.31	kJ/mol	Joback Method
hf	-352.85	kJ/mol	Joback Method
hfus	15.53	kJ/mol	Joback Method
hvap	42.62	kJ/mol	Joback Method
log10ws	-0.85		Crippen Method
logp	0.869		Crippen Method
mcvol	105.100	ml/mol	McGowan Method
pc	3965.51	kPa	Joback Method
rinpol	989.00		NIST Webbook
rinpol	992.00		NIST Webbook
rinpol	992.00		NIST Webbook
ripol	1565.00		NIST Webbook
ripol	1565.00		NIST Webbook
tb	452.95	K	Joback Method
tc	654.90	K	Joback Method
tf	254.73	K	Joback Method
vc	0.394	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.20	J/mol×K	452.95	Joback Method
cpg	213.49	J/mol×K	486.61	Joback Method
cpg	222.42	J/mol×K	520.27	Joback Method
cpg	231.01	J/mol×K	553.93	Joback Method
cpg	239.23	J/mol×K	587.58	Joback Method

cpg	247.10	J/mol×K	621.24	Joback Method
cpg	254.60	J/mol×K	654.90	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=R602563&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume