3-Sulfanylpropyl acetate

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	1000.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	1000.00		NIST Webbook
ripol	1579.00		NIST Webbook
ripol	1579.00		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=R609935&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