2-(methylthio)ethyl acetate

Inchi: InChI=1S/C5H10O2S/c1-5(6)7-3-4-8-2/h3-4H2,1-2H3
InchiKey: CQIKBSVHIBIPGY-UHFFFAOYSA-N
Formula: C5H10O2S
SMILES: CSCCOC(C)=O
Mol. weight [g/mol]: 134.20
CAS: 5862-47-5

Physical Properties

Property code	Value	Unit	Source
gf	-209.58	kJ/mol	Joback Method
hf	-349.46	kJ/mol	Joback Method
hfus	15.62	kJ/mol	Joback Method
hvap	42.70	kJ/mol	Joback Method
log10ws	-0.66		Crippen Method
logp	0.913		Crippen Method
mcvol	105.100	ml/mol	McGowan Method
pc	3740.80	kPa	Joback Method
ripol	1487.00		NIST Webbook
ripol	1538.00		NIST Webbook
ripol	1464.00		NIST Webbook
ripol	1464.00		NIST Webbook
ripol	1502.00		NIST Webbook
ripol	1490.00		NIST Webbook
ripol	1505.00		NIST Webbook
ripol	1538.00		NIST Webbook
ripol	1464.00		NIST Webbook
ripol	1505.00		NIST Webbook
ripol	1503.00		NIST Webbook
ripol	1490.00		NIST Webbook
tb	458.87	K	Joback Method
tc	660.77	K	Joback Method
tf	252.67	K	Joback Method
vc	0.394	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.45	J/mol×K	458.87	Joback Method
cpg	214.81	J/mol×K	492.52	Joback Method
cpg	223.85	J/mol×K	526.17	Joback Method
cpg	232.56	J/mol×K	559.82	Joback Method
cpg	240.93	J/mol×K	593.47	Joback Method
cpg	248.95	J/mol×K	627.12	Joback Method
cpg	256.60	J/mol×K	660.77	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=C5862475&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume