Methyl allylthioacetate

Inchi: InChI=1S/C6H10O2S/c1-3-4-9-5-6(7)8-2/h3H,1,4-5H2,2H3
InchiKey: XUIRWMWZYBMPQC-UHFFFAOYSA-N
Formula: C6H10O2S
SMILES: C=CCSCC(=O)OC
Mol. weight [g/mol]: 146.21
CAS: 72867-23-3

Physical Properties

Property code	Value	Unit	Source
gf	-113.32	kJ/mol	Joback Method
hf	-244.67	kJ/mol	Joback Method
hfus	16.93	kJ/mol	Joback Method
hvap	44.25	kJ/mol	Joback Method
log10ws	-0.93		Crippen Method
logp	1.079		Crippen Method
mcvol	114.890	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
ripol	1518.00		NIST Webbook
ripol	1518.00		NIST Webbook
tb	478.43	K	Joback Method
tc	682.10	K	Joback Method
tf	262.18	K	Joback Method
vc	0.430	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.42	J/mol×K	478.43	Joback Method
cpg	238.35	J/mol×K	512.37	Joback Method
cpg	247.88	J/mol×K	546.32	Joback Method
cpg	256.99	J/mol×K	580.26	Joback Method
cpg	265.69	J/mol×K	614.21	Joback Method
cpg	273.98	J/mol×K	648.15	Joback Method
cpg	281.84	J/mol×K	682.10	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	315.50 ± 0.50	K	0.01	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72867233&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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