

Methyl hydrogen s-acetylmercaptosuccinate

Inchi:	InChI=1S/C7H10O5S/c1-4(8)13-5(3-6(9)10)7(11)12-2/h5H,3H2,1-2H3,(H,9,10)
InchiKey:	BBFXRNQBSGBOAC-UHFFFAOYSA-N
Formula:	C7H10O5S
SMILES:	<chem>COC(=O)C(CC(=O)O)SC(C)=O</chem>
Mol. weight [g/mol]:	206.22
CAS:	88942-56-7

Physical Properties

Property code	Value	Unit	Source
gf	-589.84	kJ/mol	Joback Method
hf	-773.41	kJ/mol	Joback Method
hfus	24.57	kJ/mol	Joback Method
hvap	76.93	kJ/mol	Joback Method
log10ws	-0.49		Crippen Method
logp	0.282		Crippen Method
mcvol	142.290	ml/mol	McGowan Method
pc	3901.37	kPa	Joback Method
tb	704.11	K	Joback Method
tc	907.45	K	Joback Method
tf	420.89	K	Joback Method
vc	0.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.06	J/molxK	704.11	Joback Method
cpg	366.45	J/molxK	738.00	Joback Method
cpg	374.28	J/molxK	771.89	Joback Method
cpg	381.54	J/molxK	805.78	Joback Method
cpg	388.23	J/molxK	839.67	Joback Method
cpg	394.33	J/molxK	873.56	Joback Method
cpg	399.84	J/molxK	907.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C88942567&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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