5-acetyl-2,3-dihydro-1,4-thiazine

Other names: 5-Acetyl-2,3-dihydro-4H-1,4-thiazine
Inchi: InChI=1S/C6H9NOS/c1-5(8)6-4-9-3-2-7-6/h4,7H,2-3H2,1H3
InchiKey: YJSKAAVPUSXIPL-UHFFFAOYSA-N
Formula: C6H9NOS
SMILES: CC(=O)C1=CSCCN1
Mol. weight [g/mol]: 143.21
CAS: 101417-25-8

Physical Properties

Property code	Value	Unit	Source
gf	50.78	kJ/mol	Joback Method
hf	-75.71	kJ/mol	Joback Method
hfus	17.74	kJ/mol	Joback Method
hvap	49.96	kJ/mol	Joback Method
log10ws	-1.43		Crippen Method
logp	0.753		Crippen Method
mcvol	108.140	ml/mol	McGowan Method
pc	4736.62	kPa	Joback Method
rinpol	1372.00		NIST Webbook
tb	515.29	K	Joback Method
tc	760.38	K	Joback Method
tf	420.69	K	Joback Method
vc	0.381	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.65	J/mol×K	515.29	Joback Method
cpg	231.82	J/mol×K	556.14	Joback Method
cpg	243.24	J/mol×K	596.99	Joback Method
cpg	253.93	J/mol×K	637.83	Joback Method
cpg	263.91	J/mol×K	678.68	Joback Method
cpg	273.18	J/mol×K	719.53	Joback Method
cpg	281.78	J/mol×K	760.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C101417258&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume