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

Other names: 5-propionyl-3,4-dihydro-2H-1,4-thiazine
Inchi: InChI=1S/C7H11NOS/c1-2-7(9)6-5-10-4-3-8-6/h5,8H,2-4H2,1H3
InchiKey: HAUUYJAUWSVDFS-UHFFFAOYSA-N
Formula: C7H11NOS
SMILES: CCC(=O)C1=CSCCN1
Mol. weight [g/mol]: 157.23

Physical Properties

Property code	Value	Unit	Source
gf	59.20	kJ/mol	Joback Method
hf	-96.35	kJ/mol	Joback Method
hfus	20.33	kJ/mol	Joback Method
hvap	52.18	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	1.143		Crippen Method
mcvol	122.230	ml/mol	McGowan Method
pc	4167.71	kPa	Joback Method
rinpol	1450.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1456.00		NIST Webbook
ripol	2235.00		NIST Webbook
ripol	2235.00		NIST Webbook
ripol	2235.00		NIST Webbook
ripol	2235.00		NIST Webbook
tb	538.17	K	Joback Method
tc	778.36	K	Joback Method
tf	431.96	K	Joback Method
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.88	J/mol×K	538.17	Joback Method

cpg	276.22	J/mol×K	578.20	Joback Method
cpg	288.74	J/mol×K	618.23	Joback Method
cpg	300.46	J/mol×K	658.26	Joback Method
cpg	311.40	J/mol×K	698.29	Joback Method
cpg	321.59	J/mol×K	738.32	Joback Method
cpg	331.05	J/mol×K	778.36	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R222701&Units=SI

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