2-Hydroxy-3-propyl-2-cyclopenten-1-one

Other names: 2-Cyclopenten-1-one, 2-hydroxy-3-propyl
Inchi: InChI=1S/C8H12O2/c1-2-3-6-4-5-7(9)8(6)10/h10H,2-5H2,1H3
InchiKey: XAXYCXCTGDUBNW-UHFFFAOYSA-N
Formula: C8H12O2
SMILES: CCCC1=C(O)C(=O)CC1
Mol. weight [g/mol]: 140.18
CAS: 25684-04-2

Physical Properties

Property code	Value	Unit	Source
gf	-187.97	kJ/mol	Joback Method
hf	-382.72	kJ/mol	Joback Method
hfus	13.38	kJ/mol	Joback Method
hvap	56.51	kJ/mol	Joback Method
log10ws	-2.02		Crippen Method
logp	1.962		Crippen Method
mcvol	115.860	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
rinpol	1188.00		NIST Webbook
rinpol	1188.00		NIST Webbook
rinpol	1188.00		NIST Webbook
ripol	1891.00		NIST Webbook
ripol	1891.00		NIST Webbook
ripol	1891.00		NIST Webbook
tb	571.51	K	Joback Method
tc	773.68	K	Joback Method
tf	349.90	K	Joback Method
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.64	J/mol×K	571.51	Joback Method
cpg	293.12	J/mol×K	605.21	Joback Method

cpg	304.08	J/mol×K	638.90	Joback Method
cpg	314.52	J/mol×K	672.60	Joback Method
cpg	324.44	J/mol×K	706.29	Joback Method
cpg	333.85	J/mol×K	739.99	Joback Method
cpg	342.74	J/mol×K	773.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25684042&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume