1-Phenyl-2-ethyl-2-propen-1-one

Inchi: InChI=1S/C11H12O/c1-3-9(2)11(12)10-7-5-4-6-8-10/h4-8H,2-3H2,1H3
InchiKey: MUPSPIPPEPGJEY-UHFFFAOYSA-N
Formula: C11H12O
SMILES: C=C(CC)C(=O)c1ccccc1
Mol. weight [g/mol]: 160.21

Physical Properties

Property code	Value	Unit	Source
gf	104.52	kJ/mol	Joback Method
hf	-30.78	kJ/mol	Joback Method
hfus	17.30	kJ/mol	Joback Method
hvap	48.51	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	2.836		Crippen Method
mcvol	139.360	ml/mol	McGowan Method
pc	2976.29	kPa	Joback Method
rinpol	1285.00		NIST Webbook
tb	528.19	K	Joback Method
tc	748.37	K	Joback Method
tf	274.36	K	Joback Method
vc	0.531	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.63	J/mol×K	528.19	Joback Method
cpg	317.01	J/mol×K	564.89	Joback Method
cpg	330.44	J/mol×K	601.58	Joback Method
cpg	342.99	J/mol×K	638.28	Joback Method
cpg	354.68	J/mol×K	674.98	Joback Method
cpg	365.58	J/mol×K	711.68	Joback Method
cpg	375.72	J/mol×K	748.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R520471&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume