1-Phenyl-2-(1-methylethyl)-2-propen-1-one

Inchi: InChI=1S/C12H14O/c1-9(2)10(3)12(13)11-7-5-4-6-8-11/h4-9H,3H2,1-2H3
InchiKey: JGGXQMKYHHNJAF-UHFFFAOYSA-N
Formula: C12H14O
SMILES: C=C(C(=O)c1ccccc1)C(C)C
Mol. weight [g/mol]: 174.24

Physical Properties

Property code	Value	Unit	Source
gf	110.50	kJ/mol	Joback Method
hf	-56.70	kJ/mol	Joback Method
hfus	16.36	kJ/mol	Joback Method
hvap	50.35	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.082		Crippen Method
mcvol	153.450	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
rinpol	1351.00		NIST Webbook
rinpol	1351.00		NIST Webbook
tb	550.63	K	Joback Method
tc	771.86	K	Joback Method
tf	270.63	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.95	J/mol×K	550.63	Joback Method
cpg	364.53	J/mol×K	587.50	Joback Method
cpg	379.08	J/mol×K	624.37	Joback Method
cpg	392.66	J/mol×K	661.25	Joback Method
cpg	405.31	J/mol×K	698.12	Joback Method
cpg	417.10	J/mol×K	734.99	Joback Method
cpg	428.06	J/mol×K	771.86	Joback Method

Sources

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=R520431&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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