2,3-Dimethyl-1-phenyl-2-buten-1-one

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

Physical Properties

Property code	Value	Unit	Source
gf	96.77	kJ/mol	Joback Method
hf	-69.42	kJ/mol	Joback Method
hfus	20.06	kJ/mol	Joback Method
hvap	51.45	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.226		Crippen Method
mcvol	153.450	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
rinpol	1439.00		NIST Webbook
tb	558.43	K	Joback Method
tc	784.14	K	Joback Method
tf	268.35	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.05	J/mol×K	558.43	Joback Method
cpg	364.59	J/mol×K	596.05	Joback Method
cpg	379.07	J/mol×K	633.67	Joback Method
cpg	392.56	J/mol×K	671.29	Joback Method
cpg	405.12	J/mol×K	708.90	Joback Method
cpg	416.81	J/mol×K	746.52	Joback Method
cpg	427.70	J/mol×K	784.14	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=R520560&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