2-PROPEN-1-ONE, 2-METHYL-1-PHENYL-

Inchi: InChI=1S/C10H10O/c1-8(2)10(11)9-6-4-3-5-7-9/h3-7H,1H2,2H3
InchiKey: KJCFAQDTHMIAAN-UHFFFAOYSA-N
Formula: C10H10O
SMILES: C=C(C)C(=O)c1ccccc1
Mol. weight [g/mol]: 146.19

Physical Properties

Property code	Value	Unit	Source
af	0.4243		Cheméo Relay (1.0)
gf	96.10	kJ/mol	Joback Method
hf	-4.58	kJ/mol	Cheméo Relay (1.0)
hfus	14.71	kJ/mol	Joback Method
hvap	61.22	kJ/mol	Cheméo Relay (1.0)
ie	9.22	eV	Cheméo Relay (1.0)
log10ws	-2.49		Cheméo Relay (1.0)
logp	2.445		Crippen Method
mcvol	125.270	ml/mol	McGowan Method
pc	3314.37	kPa	Joback Method
tb	491.78	K	Cheméo Relay (1.0)
tc	711.78	K	Cheméo Relay (1.0)
tf	280.51	K	Cheméo Relay (1.0)
vc	0.459	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.43	J/mol×K	505.31	Joback Method
cpg	271.88	J/mol×K	542.65	Joback Method
cpg	284.43	J/mol×K	579.99	Joback Method
cpg	296.13	J/mol×K	617.33	Joback Method
cpg	307.00	J/mol×K	654.66	Joback Method
cpg	317.11	J/mol×K	692.00	Joback Method
cpg	326.49	J/mol×K	729.34	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C769608&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume