(Z)-4-Phenylbut-3-en-2-one

Inchi: InChI=1S/C10H10O/c1-9(11)7-8-10-5-3-2-4-6-10/h2-8H,1H3/b8-7-
InchiKey: BWHOZHOGCMHOBV-FPLPWBNLSA-N
Formula: C10H10O
SMILES: CC(=O)C=Cc1ccccc1
Mol. weight [g/mol]: 146.19

Physical Properties

Property code	Value	Unit	Source
gf	97.03	kJ/mol	Joback Method
hf	-8.56	kJ/mol	Joback Method
hfus	17.50	kJ/mol	Joback Method
hvap	46.83	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.289		Crippen Method
mcvol	125.270	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
rinpol	1261.00		NIST Webbook
tb	512.91	K	Joback Method
tc	738.22	K	Joback Method
tf	273.73	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.70	J/mol×K	512.91	Joback Method
cpg	316.88	J/mol×K	700.67	Joback Method
cpg	306.90	J/mol×K	663.11	Joback Method
cpg	296.15	J/mol×K	625.56	Joback Method
cpg	284.57	J/mol×K	588.01	Joback Method
cpg	272.10	J/mol×K	550.46	Joback Method
cpg	326.13	J/mol×K	738.22	Joback Method
dvisc	0.0002186	Pa×s	512.91	Joback Method
dvisc	0.0002801	Pa×s	473.05	Joback Method

dvisc	0.0003755	Pa×s	433.18	Joback Method
dvisc	0.0005344	Pa×s	393.32	Joback Method
dvisc	0.0008235	Pa×s	353.46	Joback Method
dvisc	0.0014163	Pa×s	313.59	Joback Method
dvisc	0.0028529	Pa×s	273.73	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R341327&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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