1-(pentamethylphenyl)ethan-1-one

Inchi: InChI=1S/C13H18O/c1-7-8(2)10(4)13(12(6)14)11(5)9(7)3/h1-6H3
InchiKey: CTTYWXDVWGKHKJ-UHFFFAOYSA-N
Formula: C13H18O
SMILES: CC(=O)c1c(C)c(C)c(C)c(C)c1C
Mol. weight [g/mol]: 190.28
CAS: 2040-01-9

Physical Properties

Property code	Value	Unit	Source
gf	-6.08	kJ/mol	Joback Method
hf	-245.05	kJ/mol	Joback Method
hfus	23.12	kJ/mol	Joback Method
hvap	56.86	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	3.431		Crippen Method
mcvol	171.840	ml/mol	McGowan Method
pc	2169.38	kPa	Joback Method
tb	602.29	K	Joback Method
tc	812.07	K	Joback Method
tf	375.22	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.55	J/mol×K	602.29	Joback Method
cpg	430.52	J/mol×K	637.25	Joback Method
cpg	444.78	J/mol×K	672.22	Joback Method
cpg	458.33	J/mol×K	707.18	Joback Method
cpg	471.18	J/mol×K	742.14	Joback Method
cpg	483.35	J/mol×K	777.10	Joback Method
cpg	494.83	J/mol×K	812.07	Joback Method
dvisc	0.0009177	Pa×s	375.22	Joback Method
dvisc	0.0006273	Pa×s	413.06	Joback Method

dvisc	0.0004571	Pa×s	450.91	Joback Method
dvisc	0.0003498	Pa×s	488.75	Joback Method
dvisc	0.0002782	Pa×s	526.60	Joback Method
dvisc	0.0002281	Pa×s	564.44	Joback Method
dvisc	0.0001918	Pa×s	602.29	Joback Method

Sources

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=C2040019&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume