1-(2,3,4,5-Tetramethylphenyl)-1-butanone

Inchi: InChI=1S/C14H20O/c1-6-7-14(15)13-8-9(2)10(3)11(4)12(13)5/h8H,6-7H2,1-5H3
InchiKey: KYCSTHBXFQOETE-UHFFFAOYSA-N
Formula: C14H20O
SMILES: CCCC(=O)c1cc(C)c(C)c(C)c1C
Mol. weight [g/mol]: 204.31
CAS: 69855-49-8

Physical Properties

Property code	Value	Unit	Source
gf	11.97	kJ/mol	Joback Method
hf	-254.22	kJ/mol	Joback Method
hfus	26.10	kJ/mol	Joback Method
hvap	58.43	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	3.903		Crippen Method
mcvol	185.930	ml/mol	McGowan Method
pc	2014.51	kPa	Joback Method
rinpol	1660.00		NIST Webbook
rinpol	1660.00		NIST Webbook
tb	620.19	K	Joback Method
tc	825.80	K	Joback Method
tf	373.97	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.97	J/mol×K	620.19	Joback Method
cpg	481.82	J/mol×K	654.46	Joback Method
cpg	496.87	J/mol×K	688.73	Joback Method
cpg	511.14	J/mol×K	723.00	Joback Method
cpg	524.64	J/mol×K	757.27	Joback Method
cpg	537.40	J/mol×K	791.53	Joback Method
cpg	549.43	J/mol×K	825.80	Joback Method

dvisc	0.0010996	Pa×s	373.97	Joback Method
dvisc	0.0007009	Pa×s	415.01	Joback Method
dvisc	0.0004844	Pa×s	456.04	Joback Method
dvisc	0.0003559	Pa×s	497.08	Joback Method
dvisc	0.0002741	Pa×s	538.12	Joback Method
dvisc	0.0002190	Pa×s	579.15	Joback Method
dvisc	0.0001803	Pa×s	620.19	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=C69855498&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