3-Butanone,1-(2,3,6-trimethylphenyl)-

Other names: 4-(2,3,6-Trimethylphenyl)-2-butanone
4-(2,3,6-Trimethylphenyl)butan-2-one
Inchi: InChI=1S/C13H18O/c1-9-5-6-10(2)13(12(9)4)8-7-11(3)14/h5-6H,7-8H2,1-4H3
InchiKey: YTAQPZUVJBPHEJ-UHFFFAOYSA-N
Formula: C13H18O
SMILES: CC(=O)CCc1c(C)ccc(C)c1C
Mol. weight [g/mol]: 190.28
CAS: 58720-40-4

Physical Properties

Property code	Value	Unit	Source
gf	13.18	kJ/mol	Joback Method
hf	-222.11	kJ/mol	Joback Method
hfus	23.90	kJ/mol	Joback Method
hvap	55.54	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.133		Crippen Method
mcvol	171.840	ml/mol	McGowan Method
pc	2231.30	kPa	Joback Method
rinpol	1445.00		NIST Webbook
rinpol	1445.00		NIST Webbook
ripol	2193.00		NIST Webbook
ripol	2193.00		NIST Webbook
tb	592.33	K	Joback Method
tc	800.18	K	Joback Method
tf	350.18	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.32	J/mol×K	592.33	Joback Method
cpg	431.75	J/mol×K	626.97	Joback Method
cpg	446.37	J/mol×K	661.61	Joback Method

cpg	460.21	J/mol×K	696.26	Joback Method
cpg	473.29	J/mol×K	730.90	Joback Method
cpg	485.63	J/mol×K	765.54	Joback Method
cpg	497.26	J/mol×K	800.18	Joback Method
dvisc	0.0013712	Pa×s	350.18	Joback Method
dvisc	0.0008401	Pa×s	390.54	Joback Method
dvisc	0.0005641	Pa×s	430.90	Joback Method
dvisc	0.0004056	Pa×s	471.25	Joback Method
dvisc	0.0003072	Pa×s	511.61	Joback Method
dvisc	0.0002423	Pa×s	551.97	Joback Method
dvisc	0.0001974	Pa×s	592.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C58720404&Units=SI
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

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