1-(3,4-Dimethylphenyl)-1-propanone

Inchi: InChI=1S/C11H14O/c1-4-11(12)10-6-5-8(2)9(3)7-10/h5-7H,4H2,1-3H3
InchiKey: CBALKMGGDUMBIJ-UHFFFAOYSA-N
Formula: C11H14O
SMILES: CCC(=O)c1ccc(C)c(C)c1
Mol. weight [g/mol]: 162.23

Physical Properties

Property code	Value	Unit	Source
gf	5.97	kJ/mol	Joback Method
hf	-169.36	kJ/mol	Joback Method
hfus	19.11	kJ/mol	Joback Method
hvap	50.43	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	2.896		Crippen Method
mcvol	143.660	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
ripol	2658.00		NIST Webbook
tb	541.59	K	Joback Method
tc	755.27	K	Joback Method
tf	315.12	K	Joback Method
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.49	J/mol×K	541.59	Joback Method
cpg	335.63	J/mol×K	577.20	Joback Method
cpg	349.01	J/mol×K	612.82	Joback Method
cpg	361.64	J/mol×K	648.43	Joback Method
cpg	373.55	J/mol×K	684.05	Joback Method
cpg	384.76	J/mol×K	719.66	Joback Method
cpg	395.29	J/mol×K	755.27	Joback Method
dvisc	0.0017381	Pa×s	315.12	Joback Method
dvisc	0.0010363	Pa×s	352.87	Joback Method

dvisc	0.0006829	Pa×s	390.61	Joback Method
dvisc	0.0004843	Pa×s	428.36	Joback Method
dvisc	0.0003631	Pa×s	466.10	Joback Method
dvisc	0.0002843	Pa×s	503.85	Joback Method
dvisc	0.0002302	Pa×s	541.59	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=R587701&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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