

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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0006829	Paxs	390.61	Joback Method
dvisc	0.0004843	Paxs	428.36	Joback Method
dvisc	0.0003631	Paxs	466.10	Joback Method
dvisc	0.0002843	Paxs	503.85	Joback Method
dvisc	0.0002302	Paxs	541.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R587701&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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