

3'-methylpropiophenone

Inchi:	InChI=1S/C10H12O/c1-3-10(11)9-6-4-5-8(2)7-9/h4-7H,3H2,1-2H3
InchiKey:	QHVNQIJBHWOZRJ-UHFFFAOYSA-N
Formula:	C10H12O
SMILES:	CCC(=O)c1cccc(C)c1
Mol. weight [g/mol]:	148.20
CAS:	51772-30-6

Physical Properties

Property code	Value	Unit	Source
gf	7.18	kJ/mol	Joback Method
hf	-137.25	kJ/mol	Joback Method
hfus	16.91	kJ/mol	Joback Method
hvap	47.54	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.588		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
pc	3089.85	kPa	Joback Method
tb	513.73	K	Joback Method
tc	729.82	K	Joback Method
tf	291.33	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.66	J/mol×K	513.73	Joback Method
cpg	336.91	J/mol×K	693.81	Joback Method
cpg	326.32	J/mol×K	657.79	Joback Method
cpg	315.02	J/mol×K	621.78	Joback Method
cpg	303.00	J/mol×K	585.76	Joback Method
cpg	290.22	J/mol×K	549.75	Joback Method
cpg	346.84	J/mol×K	729.82	Joback Method
dvisc	0.0002503	Pa×s	513.73	Joback Method
dvisc	0.0003132	Pa×s	476.66	Joback Method

dvisc	0.0004070	Pa×s	439.60	Joback Method
dvisc	0.0005549	Pa×s	402.53	Joback Method
dvisc	0.0008058	Pa×s	365.46	Joback Method
dvisc	0.0012729	Pa×s	328.40	Joback Method
dvisc	0.0022588	Pa×s	291.33	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	507.20	K	99.30	NIST Webbook
tbrp	405.70	K	4.00	NIST Webbook

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=C51772306&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf: Normal melting (fusion) point
vc: Critical Volume

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