p-Propylacetophenone

Other names:	p-Propylacetophenone
	p-n-Propylacetophenone
	4'-Propylacetophenone
	Ethanone, 1-(4-propylphenyl)-
	1-(4-propylphenyl)ethan-1-one
Inchi:	InChI=1S/C11H14O/c1-3-4-10-5-7-11(8-6-10)9(2)12/h5-8H,3-4H2,1-2H3
InchiKey:	ZNBVIYMIVFKTIW-UHFFFAOYSA-N
Formula:	C11H14O
SMILES:	CCCc1ccc(C(C)=O)cc1
Mol. weight [g/mol]:	162.23

Physical Properties

Property code	Value	Unit	Source
af	0.5201		Cheméo Relay (1.0)
gf	15.60	kJ/mol	Joback Method
hf	-176.06	kJ/mol	Cheméo Relay (1.0)
hfus	19.50	kJ/mol	Joback Method
hvap	69.41	kJ/mol	Cheméo Relay (1.0)
ie	9.10	eV	Cheméo Relay (1.0)
log10ws	-3.31		Cheméo Relay (1.0)
logp	2.842		Crippen Method
mcvol	143.660	ml/mol	McGowan Method
pc	2784.72	kPa	Joback Method
tb	527.00	K	Cheméo Relay (1.0)
tc	730.74	K	Cheméo Relay (1.0)
tf	283.30	K	Cheméo Relay (1.0)
vc	0.534	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.61	J/mol×K	536.61	Joback Method
cpg	336.08	J/mol×K	572.04	Joback Method
cpg	349.73	J/mol×K	607.47	Joback Method

cpg	362.58	J/mol×K	642.90	Joback Method
cpg	374.66	J/mol×K	678.33	Joback Method
cpg	386.00	J/mol×K	713.76	Joback Method
cpg	396.64	J/mol×K	749.19	Joback Method
dvisc	0.0022892	Pa×s	302.60	Joback Method
dvisc	0.0012638	Pa×s	341.60	Joback Method
dvisc	0.0007880	Pa×s	380.60	Joback Method
dvisc	0.0005365	Pa×s	419.60	Joback Method
dvisc	0.0003899	Pa×s	458.61	Joback Method
dvisc	0.0002979	Pa×s	497.61	Joback Method
dvisc	0.0002367	Pa×s	536.61	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	429.50 ± 1.50	K	2.40	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2932652&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor

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
ie:	Ionization energy
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