

p-n-Butylacetophenone

Other names:	Ethanone, 1-(4-butylphenyl)- p-Butylacetophenone 1-(4-butylphenyl)ethan-1-one
Inchi:	InChI=1S/C12H16O/c1-3-4-5-11-6-8-12(9-7-11)10(2)13/h6-9H,3-5H2,1-2H3
InchiKey:	MQESVSITPLILCO-UHFFFAOYSA-N
Formula:	C12H16O
SMILES:	CCCCc1ccc(C(C)=O)cc1
Mol. weight [g/mol]:	176.25
CAS:	37920-25-5

Physical Properties

Property code	Value	Unit	Source
gf	24.02	kJ/mol	Joback Method
hf	-178.53	kJ/mol	Joback Method
hfus	22.09	kJ/mol	Joback Method
hvap	51.99	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.232		Crippen Method
mcvol	157.750	ml/mol	McGowan Method
pc	2522.65	kPa	Joback Method
tb	559.49	K	Joback Method
tc	768.65	K	Joback Method
tf	313.87	K	Joback Method
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.35	J/molxK	559.49	Joback Method
cpg	436.31	J/molxK	733.79	Joback Method
cpg	424.32	J/molxK	698.93	Joback Method
cpg	411.56	J/molxK	664.07	Joback Method
cpg	398.00	J/molxK	629.21	Joback Method
cpg	383.60	J/molxK	594.35	Joback Method

cpg	447.57	J/molxK	768.65	Joback Method
dvisc	0.0002212	Paxs	559.49	Joback Method
dvisc	0.0002799	Paxs	518.55	Joback Method
dvisc	0.0003688	Paxs	477.62	Joback Method
dvisc	0.0005117	Paxs	436.68	Joback Method
dvisc	0.0007598	Paxs	395.74	Joback Method
dvisc	0.0012360	Paxs	354.81	Joback Method
dvisc	0.0022825	Paxs	313.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C37920255&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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