

p-Octylacetophenone

Other names:	4-n-Octylacetophenone p-n-Octylacetophenone Acetophenone, 4'-octyl- Ethanone, 1-(4-octylphenyl)- 4'-Octylacetophenone
Inchi:	InChI=1S/C16H24O/c1-3-4-5-6-7-8-9-15-10-12-16(13-11-15)14(2)17/h10-13H,3-9H2,1-2
InchiKey:	GARQDIVXKVBJFP-UHFFFAOYSA-N
Formula:	C16H24O
SMILES:	CCCCCCCCc1ccc(C(C)=O)cc1
Mol. weight [g/mol]:	232.36
CAS:	10541-56-7

Physical Properties

Property code	Value	Unit	Source
gf	57.70	kJ/mol	Joback Method
hf	-261.09	kJ/mol	Joback Method
hfus	32.45	kJ/mol	Joback Method
hvap	60.89	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	4.792		Crippen Method
mcvol	214.110	ml/mol	McGowan Method
pc	1772.85	kPa	Joback Method
tb	651.01	K	Joback Method
tc	848.49	K	Joback Method
tf	358.95	K	Joback Method
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.23	J/molxK	651.01	Joback Method
cpg	648.98	J/molxK	815.58	Joback Method
cpg	635.20	J/molxK	782.66	Joback Method
cpg	620.57	J/molxK	749.75	Joback Method

cpg	605.06	J/molxK	716.84	Joback Method
cpg	588.62	J/molxK	683.92	Joback Method
cpg	661.95	J/molxK	848.49	Joback Method
dvisc	0.0001543	Paxs	651.01	Joback Method
dvisc	0.0001988	Paxs	602.33	Joback Method
dvisc	0.0002680	Paxs	553.66	Joback Method
dvisc	0.0003827	Paxs	504.98	Joback Method
dvisc	0.0005895	Paxs	456.30	Joback Method
dvisc	0.0010068	Paxs	407.63	Joback Method
dvisc	0.0019882	Paxs	358.95	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	425.50 ± 0.50	K	0.10	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10541567&Units=SI
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

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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