2-Naphthyl phenyl ketone

Other names: 2-Benzoylnaphthalene
«beta»-Naphthyl phenyl ketone
2-Naphthyl phenyl ketone
«beta»-Benzoylnaphthalene
Ketone, 2-naphthyl phenyl
2-Benzonaphthone
2'-benzonaphthone

Inchi: InChI=1S/C17H12O/c18-17(14-7-2-1-3-8-14)16-11-10-13-6-4-5-9-15(13)12-16/h1-12H

InchiKey: SJNXJRVDSTZUFB-UHFFFAOYSA-N

Formula: C17H12O

SMILES: O=C(c1ccccc1)c1ccc2ccccc2c1

Mol. weight [g/mol]: 232.28

Physical Properties

Property code	Value	Unit	Source
af	0.5790		Cheméo Relay (1.0)
gf	285.18	kJ/mol	Joback Method
hf	119.19	kJ/mol	Cheméo Relay (1.0)
hfus	26.10	kJ/mol	Joback Method
hvap	109.41	kJ/mol	Cheméo Relay (1.0)
ie	8.36	eV	Cheméo Relay (1.0)
log10ws	-5.27		Cheméo Relay (1.0)
logp	4.071		Crippen Method
mcvol	184.980	ml/mol	McGowan Method
pc	2784.72	kPa	Joback Method
tb	665.94	K	Cheméo Relay (1.0)
tc	962.79	K	Cheméo Relay (1.0)
tf	395.73	K	Cheméo Relay (1.0)
vc	0.685	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	478.05	J/mol×K	719.55	Joback Method

cpg	493.00	J/mol×K	763.16	Joback Method
cpg	506.61	J/mol×K	806.76	Joback Method
cpg	519.02	J/mol×K	850.37	Joback Method
cpg	530.39	J/mol×K	893.98	Joback Method
cpg	540.84	J/mol×K	937.58	Joback Method
cpg	550.54	J/mol×K	981.19	Joback Method
dvisc	0.0014855	Pa×s	429.34	Joback Method
dvisc	0.0009545	Pa×s	477.71	Joback Method
dvisc	0.0006653	Pa×s	526.08	Joback Method
dvisc	0.0004928	Pa×s	574.44	Joback Method
dvisc	0.0003824	Pa×s	622.81	Joback Method
dvisc	0.0003078	Pa×s	671.18	Joback Method
dvisc	0.0002551	Pa×s	719.55	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C644133&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

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