

1-(2-naphthyl)propan-1-one

Inchi:	InChI=1S/C13H12O/c1-2-13(14)12-8-7-10-5-3-4-6-11(10)9-12/h3-9H,2H2,1H3
InchiKey:	QLYPHTMKMPIJNG-UHFFFAOYSA-N
Formula:	C13H12O
SMILES:	CCC(=O)c1ccc2ccccc2c1
Mol. weight [g/mol]:	184.23
CAS:	6315-96-4

Physical Properties

Property code	Value	Unit	Source
gf	139.09	kJ/mol	Joback Method
hf	-8.10	kJ/mol	Joback Method
hfus	21.70	kJ/mol	Joback Method
hvap	55.86	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	3.433		Crippen Method
mcvol	152.380	ml/mol	McGowan Method
pc	2947.28	kPa	Joback Method
tb	586.20	K	NIST Webbook
tc	835.25	K	Joback Method
tf	357.84	K	Joback Method
vc	0.584	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.21	J/mol×K	601.35	Joback Method
cpg	374.56	J/mol×K	640.33	Joback Method
cpg	387.85	J/mol×K	679.32	Joback Method
cpg	400.15	J/mol×K	718.30	Joback Method
cpg	411.54	J/mol×K	757.29	Joback Method
cpg	422.09	J/mol×K	796.27	Joback Method
cpg	431.89	J/mol×K	835.25	Joback Method
dvisc	0.0017698	Pa×s	357.84	Joback Method
dvisc	0.0011662	Pa×s	398.43	Joback Method

dvisc	0.0008301	Pa×s	439.01	Joback Method
dvisc	0.0006258	Pa×s	479.60	Joback Method
dvisc	0.0004931	Pa×s	520.18	Joback Method
dvisc	0.0004021	Pa×s	560.77	Joback Method
dvisc	0.0003371	Pa×s	601.35	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	455.20	K	2.40	NIST Webbook

Sources

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=C6315964&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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