

2(1H)-Naphthalenone, 4-methyl

Inchi:

InChI=1S/C11H10O/c1-8-6-10(12)7-9-4-2-3-5-11(8)9/h2-6H,7H2,1H3

InchiKey:

FLCQYXWYKZDWKF-UHFFFAOYSA-N

Formula:

C11H10O

SMILES:

CC1=CC(=O)Cc2ccccc21

Mol. weight [g/mol]:

158.20

Physical Properties

Property code	Value	Unit	Source
gf	98.62	kJ/mol	Joback Method
hf	-49.72	kJ/mol	Joback Method
hfus	13.21	kJ/mol	Joback Method
hvap	48.61	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.215		Crippen Method
mcvol	128.500	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
rinpol	1514.00		NIST Webbook
tb	570.38	K	Joback Method
tc	818.31	K	Joback Method
tf	352.83	K	Joback Method
vc	0.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.72	J/mol×K	570.38	Joback Method
cpg	309.50	J/mol×K	611.70	Joback Method
cpg	323.29	J/mol×K	653.02	Joback Method
cpg	336.12	J/mol×K	694.35	Joback Method
cpg	348.04	J/mol×K	735.67	Joback Method
cpg	359.07	J/mol×K	776.99	Joback Method
cpg	369.26	J/mol×K	818.31	Joback Method

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=R71836&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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