2(1H)-Naphthalenone, 1-methyl

Inchi: InChI=1S/C11H10O/c1-8-10-5-3-2-4-9(10)6-7-11(8)12/h2-8H,1H3
InchiKey: KBYAXHYSPYSWSO-UHFFFAOYSA-N
Formula: C11H10O
SMILES: CC1C(=O)C=Cc2ccccc21
Mol. weight [g/mol]: 158.20

Physical Properties

Property code	Value	Unit	Source
gf	100.54	kJ/mol	Joback Method
hf	-58.59	kJ/mol	Joback Method
hfus	14.66	kJ/mol	Joback Method
hvap	47.64	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	2.386		Crippen Method
mcvol	128.500	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
rinpol	1479.00		NIST Webbook
tb	560.73	K	Joback Method
tc	807.61	K	Joback Method
tf	336.07	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	297.03	J/mol×K	560.73	Joback Method
cpg	312.64	J/mol×K	601.88	Joback Method
cpg	327.21	J/mol×K	643.02	Joback Method
cpg	340.76	J/mol×K	684.17	Joback Method
cpg	353.33	J/mol×K	725.32	Joback Method
cpg	364.95	J/mol×K	766.46	Joback Method
cpg	375.66	J/mol×K	807.61	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=R71822&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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