2(1H)-Naphthalenone, 7-methoxy

Inchi: InChI=1S/C11H10O2/c1-13-11-5-3-8-2-4-10(12)6-9(8)7-11/h2-5,7H,6H2,1H3
InchiKey: MINAMHVSKCELFL-UHFFFAOYSA-N
Formula: C11H10O2
SMILES: COc1ccc2c(c1)CC(=O)C=C2
Mol. weight [g/mol]: 174.20

Physical Properties

Property code	Value	Unit	Source
gf	-6.38	kJ/mol	Joback Method
hf	-181.94	kJ/mol	Joback Method
hfus	14.39	kJ/mol	Joback Method
hvap	51.02	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	1.834		Crippen Method
mcvol	134.370	ml/mol	McGowan Method
pc	3337.38	kPa	Joback Method
rinpol	1680.00		NIST Webbook
tb	592.80	K	Joback Method
tc	836.85	K	Joback Method
tf	375.06	K	Joback Method
vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.49	J/mol×K	592.80	Joback Method
cpg	332.96	J/mol×K	633.48	Joback Method
cpg	346.52	J/mol×K	674.15	Joback Method
cpg	359.17	J/mol×K	714.83	Joback Method
cpg	370.92	J/mol×K	755.50	Joback Method
cpg	381.79	J/mol×K	796.18	Joback Method
cpg	391.80	J/mol×K	836.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R71854&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
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