3-Methyl-9-fluorenone

Inchi: InChI=1S/C14H10O/c1-9-6-7-12-13(8-9)10-4-2-3-5-11(10)14(12)15/h2-8H,1H3
InchiKey: CCPOGGQELUULQK-UHFFFAOYSA-N
Formula: C14H10O
SMILES: Cc1ccc2c(c1)-c1ccccc1C2=O
Mol. weight [g/mol]: 194.23
CAS: 1705-89-1

Physical Properties

Property code	Value	Unit	Source
gf	233.00	kJ/mol	Joback Method
hf	74.12	kJ/mol	Joback Method
hfus	19.71	kJ/mol	Joback Method
hvap	57.42	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	3.206		Crippen Method
mcvol	151.310	ml/mol	McGowan Method
pc	3096.73	kPa	Joback Method
tb	658.71	K	Joback Method
tc	914.85	K	Joback Method
tf	435.38	K	Joback Method
vc	0.585	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.42	J/mol×K	658.71	Joback Method
cpg	390.41	J/mol×K	701.40	Joback Method
cpg	403.34	J/mol×K	744.09	Joback Method
cpg	415.31	J/mol×K	786.78	Joback Method
cpg	426.42	J/mol×K	829.47	Joback Method
cpg	436.76	J/mol×K	872.16	Joback Method
cpg	446.42	J/mol×K	914.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1705891&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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