4-methylindanone

Inchi: InChI=1S/C10H10O/c1-7-3-2-4-9-8(7)5-6-10(9)11/h2-4H,5-6H2,1H3
InchiKey: RUORWXQKVXTQJJ-UHFFFAOYSA-N
Formula: C10H10O
SMILES: Cc1cccc2c1CCC2=O
Mol. weight [g/mol]: 146.19
CAS: 24644-78-8

Physical Properties

Property code	Value	Unit	Source
gf	72.34	kJ/mol	Joback Method
hf	-80.70	kJ/mol	Joback Method
hfus	11.49	kJ/mol	Joback Method
hvap	45.92	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.124		Crippen Method
mcvol	118.710	ml/mol	McGowan Method
pc	3547.31	kPa	Joback Method
rinpol	1444.00		NIST Webbook
tb	544.07	K	Joback Method
tc	785.60	K	Joback Method
tf	344.32	K	Joback Method
vc	0.453	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.86	J/mol×K	544.07	Joback Method
cpg	282.04	J/mol×K	584.33	Joback Method
cpg	295.31	J/mol×K	624.58	Joback Method
cpg	307.73	J/mol×K	664.84	Joback Method
cpg	319.32	J/mol×K	705.09	Joback Method
cpg	330.13	J/mol×K	745.35	Joback Method
cpg	340.20	J/mol×K	785.60	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=C24644788&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