4-Methyl-3-vinyl-3-cyclohexen-1-one

Inchi: InChI=1S/C9H12O/c1-3-8-6-9(10)5-4-7(8)2/h3H,1,4-6H2,2H3
InchiKey: IHAUJYOJZSPIFG-UHFFFAOYSA-N
Formula: C9H12O
SMILES: C=CC1=C(C)CCC(=O)C1
Mol. weight [g/mol]: 136.19

Physical Properties

Property code	Value	Unit	Source
gf	33.01	kJ/mol	Joback Method
hf	-131.86	kJ/mol	Joback Method
hfus	8.50	kJ/mol	Joback Method
hvap	41.56	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	2.242		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3224.64	kPa	Joback Method
rinpol	1146.00		NIST Webbook
rinpol	1146.00		NIST Webbook
tb	503.16	K	Joback Method
tc	730.05	K	Joback Method
tf	295.07	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.80	J/mol×K	503.16	Joback Method
cpg	271.68	J/mol×K	540.97	Joback Method
cpg	285.85	J/mol×K	578.79	Joback Method
cpg	299.31	J/mol×K	616.60	Joback Method
cpg	312.06	J/mol×K	654.42	Joback Method
cpg	324.10	J/mol×K	692.23	Joback Method
cpg	335.43	J/mol×K	730.05	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=R589490&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