Cycloionone

Inchi: InChI=1S/C13H20O/c1-10-6-7-11-12(2,3)8-5-9-13(11,4)14-10/h6-7H,5,8-9H2,1-4H3
InchiKey: KYOSLSFHZKIUEM-UHFFFAOYSA-N
Formula: C13H20O
SMILES: CC1=CC=C2C(C)(C)CCCC2(C)O1
Mol. weight [g/mol]: 192.30

Physical Properties

Property code	Value	Unit	Source
gf	75.24	kJ/mol	Joback Method
hf	-199.59	kJ/mol	Joback Method
hfus	14.34	kJ/mol	Joback Method
hvap	49.16	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.816		Crippen Method
mcvol	169.580	ml/mol	McGowan Method
pc	2543.05	kPa	Joback Method
ripol	1628.00		NIST Webbook
ripol	1628.00		NIST Webbook
tb	563.11	K	Joback Method
tc	797.62	K	Joback Method
tf	359.00	K	Joback Method
vc	0.634	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.46	J/mol×K	563.11	Joback Method
cpg	451.09	J/mol×K	602.20	Joback Method
cpg	469.38	J/mol×K	641.28	Joback Method
cpg	486.60	J/mol×K	680.37	Joback Method
cpg	503.01	J/mol×K	719.45	Joback Method
cpg	518.91	J/mol×K	758.54	Joback Method
cpg	534.55	J/mol×K	797.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R327212&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume