Cyclotridecanone

Inchi: InChI=1S/C13H24O/c14-13-11-9-7-5-3-1-2-4-6-8-10-12-13/h1-12H2
InchiKey: VHUGWUBIUBBUAF-UHFFFAOYSA-N
Formula: C13H24O
SMILES: O=C1CCCCCCCCCCCC1
Mol. weight [g/mol]: 196.33
CAS: 832-10-0

Physical Properties

Property code	Value	Unit	Source
gf	-116.55	kJ/mol	Joback Method
hf	-417.81	kJ/mol	Joback Method
hfus	5.00	kJ/mol	Joback Method
hvap	50.72	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	4.250		Crippen Method
mcvol	184.740	ml/mol	McGowan Method
pc	2455.60	kPa	Joback Method
rinpol	1677.80		NIST Webbook
rinpol	1672.80		NIST Webbook
rinpol	1647.60		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1661.30		NIST Webbook
tb	618.77	K	Joback Method
tc	877.46	K	Joback Method
tf	291.47	K	Joback Method
vc	0.648	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.36	J/mol×K	618.77	Joback Method
cpg	531.69	J/mol×K	661.88	Joback Method
cpg	558.04	J/mol×K	705.00	Joback Method
cpg	582.35	J/mol×K	748.11	Joback Method

cpg	604.55	J/mol×K	791.23	Joback Method
cpg	624.57	J/mol×K	834.34	Joback Method
cpg	642.34	J/mol×K	877.46	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	419.20	K	1.50	NIST Webbook

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=C832100&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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume