Cyclodecanone

Inchi: InChI=1S/C10H18O/c11-10-8-6-4-2-1-3-5-7-9-10/h1-9H2
InchiKey: SXOZDDAFVJANJP-UHFFFAOYSA-N
Formula: C10H18O
SMILES: O=C1CCCCCCCCC1
Mol. weight [g/mol]: 154.25
CAS: 1502-06-3

Physical Properties

Property code	Value	Unit	Source
chl	-6144.30 ± 1.70	kJ/mol	NIST Webbook
chl	-6166.40	kJ/mol	NIST Webbook
gf	-105.51	kJ/mol	Joback Method
hf	-305.10 ± 1.90	kJ/mol	NIST Webbook
hfl	-363.40 ± 1.80	kJ/mol	NIST Webbook
hfus	3.53	kJ/mol	Joback Method
hvap	58.37 ± 0.63	kJ/mol	NIST Webbook
hvap	58.40 ± 0.60	kJ/mol	NIST Webbook
ie	9.19	eV	NIST Webbook
log10ws	-3.18		Crippen Method
logp	3.080		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	3069.34	kPa	Joback Method
rinpol	1380.30		NIST Webbook
rinpol	1380.30		NIST Webbook
rinpol	1390.60		NIST Webbook
rinpol	1378.50		NIST Webbook
rinpol	1375.70		NIST Webbook
rinpol	1369.70		NIST Webbook
ripol	1726.00		NIST Webbook
ripol	1723.00		NIST Webbook
ripol	1744.00		NIST Webbook
ripol	1726.00		NIST Webbook
ripol	1723.00		NIST Webbook
tb	509.20 ± 1.50	K	NIST Webbook
tc	785.28	K	Joback Method
tf	296.00 ± 0.10	K	NIST Webbook
vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.10	J/mol×K	743.96	Joback Method
cpg	340.44	J/mol×K	537.32	Joback Method
cpg	363.63	J/mol×K	578.65	Joback Method
cpg	385.53	J/mol×K	619.97	Joback Method
cpg	406.10	J/mol×K	661.30	Joback Method
cpg	425.30	J/mol×K	702.63	Joback Method
cpg	459.46	J/mol×K	785.28	Joback Method
hfust	24.30	kJ/mol	294.90	NIST Webbook
hfust	24.30	kJ/mol	294.90	NIST Webbook
hvapt	55.20	kJ/mol	388.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	379.70	K	1.60	NIST Webbook
tbrp	379.00	K	1.60	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1502063&Units=SI

Legend

chl: Standard liquid enthalpy of combustion

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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
ripol:	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