Cycloundecanone

Inchi: InChI=1S/C11H20O/c12-11-9-7-5-3-1-2-4-6-8-10-11/h1-10H2
InchiKey: UPOSSYJVWXLPTA-UHFFFAOYSA-N
Formula: C11H20O
SMILES: O=C1CCCCCCCCCC1
Mol. weight [g/mol]: 168.28
CAS: 878-13-7

Physical Properties

Property code	Value	Unit	Source
chl	-6800.70 ± 2.00	kJ/mol	NIST Webbook
gf	-109.19	kJ/mol	Joback Method
hf	-322.00 ± 2.20	kJ/mol	NIST Webbook
hfl	-386.40 ± 2.10	kJ/mol	NIST Webbook
hfus	4.02	kJ/mol	Joback Method
hvap	64.30 ± 0.60	kJ/mol	NIST Webbook
hvap	64.35 ± 0.63	kJ/mol	NIST Webbook
log10ws	-3.60		Crippen Method
logp	3.470		Crippen Method
mcvol	156.560	ml/mol	McGowan Method
pc	2841.41	kPa	Joback Method
rinpol	1488.50		NIST Webbook
rinpol	1483.90		NIST Webbook
rinpol	1471.90		NIST Webbook
rinpol	1474.40		NIST Webbook
rinpol	1465.40		NIST Webbook
rinpol	1474.40		NIST Webbook
tb	520.30 ± 1.50	K	NIST Webbook
tc	816.39	K	Joback Method
tf	275.97	K	Joback Method
vc	0.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	440.92	J/mol×K	648.44	Joback Method
cpg	462.97	J/mol×K	690.43	Joback Method
cpg	483.43	J/mol×K	732.42	Joback Method
cpg	502.25	J/mol×K	774.41	Joback Method
cpg	392.21	J/mol×K	564.47	Joback Method
cpg	417.31	J/mol×K	606.46	Joback Method
cpg	519.37	J/mol×K	816.39	Joback Method
hfust	23.00	kJ/mol	287.70	NIST Webbook
hfust	23.00	kJ/mol	287.70	NIST Webbook
hvapt	60.30	kJ/mol	398.00	NIST Webbook
hvapt	51.80	kJ/mol	474.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	379.20	K	0.50	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=C878137&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
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