Cyclododecanone

Inchi: InChI=1S/C12H22O/c13-12-10-8-6-4-2-1-3-5-7-9-11-12/h1-11H2
InchiKey: SXVPOSFURRDKBO-UHFFFAOYSA-N
Formula: C12H22O
SMILES: O=C1CCCCCCCCCCC1
Mol. weight [g/mol]: 182.30
CAS: 830-13-7

Physical Properties

Property code	Value	Unit	Source
chs	-7436.10 ± 2.60	kJ/mol	NIST Webbook
chs	-7435.10 ± 2.10	kJ/mol	NIST Webbook
gf	-112.87	kJ/mol	Joback Method
hf	-349.10 ± 2.30	kJ/mol	NIST Webbook
hf	-359.30 ± 3.10	kJ/mol	NIST Webbook
hfs	-431.30 ± 2.20	kJ/mol	NIST Webbook
hfs	-442.50 ± 3.10	kJ/mol	NIST Webbook
hfus	4.51	kJ/mol	Joback Method
hsub	83.20 ± 0.30	kJ/mol	NIST Webbook
hsub	83.20 ± 0.30	kJ/mol	NIST Webbook
hvap	65.50 ± 0.60	kJ/mol	NIST Webbook
ie	8.96 ± 0.03	eV	NIST Webbook
log10ws	-4.02		Crippen Method
logp	3.860		Crippen Method
mcvol	170.650	ml/mol	McGowan Method
pc	2637.96	kPa	Joback Method
rinpol	1492.80		NIST Webbook
rinpol	1524.00		NIST Webbook
rinpol	1492.80		NIST Webbook
rinpol	1524.00		NIST Webbook
rinpol	1574.10		NIST Webbook
rinpol	1505.60		NIST Webbook
rinpol	1528.90		NIST Webbook
rinpol	1570.40		NIST Webbook
rinpol	1528.90		NIST Webbook
rinpol	1505.60		NIST Webbook
rinpol	1562.80		NIST Webbook
rinpol	1524.00		NIST Webbook

ripol	1992.70		NIST Webbook
ripol	1923.20		NIST Webbook
ripol	1956.40		NIST Webbook
ripol	1992.70		NIST Webbook
ripol	1956.40		NIST Webbook
ripol	1923.20		NIST Webbook
tb	538.30 ± 2.00	K	NIST Webbook
tc	847.11	K	Joback Method
tf	335.60 ± 0.10	K	NIST Webbook
vc	0.601	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.50	J/mol×K	676.78	Joback Method
cpg	521.80	J/mol×K	719.36	Joback Method
cpg	543.27	J/mol×K	761.94	Joback Method
cpg	562.83	J/mol×K	804.52	Joback Method
cpg	446.58	J/mol×K	591.62	Joback Method
cpg	473.40	J/mol×K	634.20	Joback Method
cpg	580.44	J/mol×K	847.11	Joback Method
hfust	16.85	kJ/mol	335.60	NIST Webbook
hvapt	61.00	kJ/mol	408.00	NIST Webbook
hvapt	57.90	kJ/mol	429.00	NIST Webbook
hvapt	54.70	kJ/mol	507.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	358.20	K	0.10	NIST Webbook
tbrp	358.00	K	0.10	NIST Webbook

Sources

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=C830137&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
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