

Cyclopentadecanone

Other names:	Exaltone
	Normuscon
	Normuscone
Inchi:	InChI=1S/C15H28O/c16-15-13-11-9-7-5-3-1-2-4-6-8-10-12-14-15/h1-14H2
InchiKey:	OSOIQJGOYGSIMF-UHFFFAOYSA-N
Formula:	C15H28O
SMILES:	O=C1CCCCCCCCCCCCCCC1
Mol. weight [g/mol]:	224.38
CAS:	502-72-7

Physical Properties

Property code	Value	Unit	Source
chs	-9412.30 ± 9.20	kJ/mol	NIST Webbook
gf	-123.91	kJ/mol	Joback Method
hf	-471.41	kJ/mol	Joback Method
hfus	5.98	kJ/mol	Joback Method
hvap	55.52	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	5.031		Crippen Method
mcvol	212.920	ml/mol	McGowan Method
pc	2143.35	kPa	Joback Method
rinpol	1845.50		NIST Webbook
rinpol	1851.70		NIST Webbook
rinpol	1862.00		NIST Webbook
rinpol	1860.90		NIST Webbook
rinpol	1840.20		NIST Webbook
tb	673.07	K	Joback Method
tc	937.23	K	Joback Method
tf	306.97	K	Joback Method
vc	0.745	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	623.39	J/mol×K	673.07	Joback Method
cpg	653.99	J/mol×K	717.10	Joback Method
cpg	682.07	J/mol×K	761.12	Joback Method
cpg	707.55	J/mol×K	805.15	Joback Method
cpg	730.34	J/mol×K	849.18	Joback Method
cpg	750.34	J/mol×K	893.20	Joback Method
cpg	767.47	J/mol×K	937.23	Joback Method
hsubt	86.00 ± 0.60	kJ/mol	305.50	NIST Webbook
hsubt	77.40 ± 0.80	kJ/mol	321.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	393.20	K	0.04	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C502727&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

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
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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

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