Cyclotetradecane

Inchi: InChI=1S/C14H28/c1-2-4-6-8-10-12-14-13-11-9-7-5-3-1/h1-14H2
InchiKey: KATXJJSCAPBIOB-UHFFFAOYSA-N
Formula: C14H28
SMILES: C1CCCCCCCCCCCCC1
Mol. weight [g/mol]: 196.37
CAS: 295-17-0

Physical Properties

Property code	Value	Unit	Source
chs	-9136.50 ± 1.30	kJ/mol	NIST Webbook
chs	-9138.70 ± 3.70	kJ/mol	NIST Webbook
gf	2.36	kJ/mol	Joback Method
hf	-239.20 ± 2.30	kJ/mol	NIST Webbook
hfs	-372.10 ± 4.10	kJ/mol	NIST Webbook
hfus	5.98	kJ/mol	Joback Method
hsub	95.60	kJ/mol	NIST Webbook
hsub	132.90	kJ/mol	NIST Webbook
hvap	65.30 ± 0.20	kJ/mol	NIST Webbook
log10ws	-5.58		Crippen Method
logp	5.461		Crippen Method
mcvol	197.260	ml/mol	McGowan Method
pc	2216.62	kPa	Joback Method
rinpol	1673.00		NIST Webbook
rinpol	1673.00		NIST Webbook
rinpol	1669.00		NIST Webbook
rinpol	1677.00		NIST Webbook
tb	578.10	K	Joback Method
tc	826.45	K	Joback Method
tf	329.00 ± 0.30	K	NIST Webbook
tf	325.00 ± 3.00	K	NIST Webbook
tf	330.00 ± 1.00	K	NIST Webbook
vc	0.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.24	J/mol×K	578.10	Joback Method
cpg	573.62	J/mol×K	660.88	Joback Method
cpg	669.78	J/mol×K	826.45	Joback Method
cpg	600.76	J/mol×K	702.27	Joback Method
cpg	625.85	J/mol×K	743.66	Joback Method
cpg	648.86	J/mol×K	785.06	Joback Method
cpg	544.43	J/mol×K	619.49	Joback Method
dvisc	0.0000469	Pa×s	520.25	Joback Method
dvisc	0.0001144	Pa×s	462.40	Joback Method
dvisc	0.0003601	Pa×s	404.55	Joback Method
dvisc	0.0016616	Pa×s	346.70	Joback Method
dvisc	0.0141473	Pa×s	288.85	Joback Method
dvisc	0.0000230	Pa×s	578.10	Joback Method
dvisc	0.3521345	Pa×s	231.00	Joback Method
hfust	28.70	kJ/mol	328.00	NIST Webbook
hfust	28.70	kJ/mol	328.00	NIST Webbook
hsubt	134.80 ± 1.50	kJ/mol	355.00	NIST Webbook
hsubt	89.30 ± 0.40	kJ/mol	287.50	NIST Webbook
hsubt	134.80 ± 1.50	kJ/mol	301.00	NIST Webbook
hsubt	97.90 ± 1.70	kJ/mol	310.50	NIST Webbook
hvapt	62.30 ± 0.20	kJ/mol	343.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40625e+01
Coeff. B	-4.30467e+03
Coeff. C	-8.56400e+01
Temperature range (K), min.	398.14
Temperature range (K), max.	577.55

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C295170&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
dvisc:	Dynamic viscosity
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
hsubt:	Enthalpy of sublimation 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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume