Cyclotridecane

Inchi: InChI=1S/C13H26/c1-2-4-6-8-10-12-13-11-9-7-5-3-1/h1-13H2
InchiKey: UEVXKGPJXXDGCX-UHFFFAOYSA-N
Formula: C13H26
SMILES: C1CCCCCCCCCCCC1
Mol. weight [g/mol]: 182.35
CAS: 295-02-3

Physical Properties

Property code	Value	Unit	Source
chl	-8521.80 ± 1.50	kJ/mol	NIST Webbook
gf	6.04	kJ/mol	Joback Method
hf	-280.11	kJ/mol	Joback Method
hfus	5.49	kJ/mol	Joback Method
hvap	46.47	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	5.071		Crippen Method
mcvol	183.170	ml/mol	McGowan Method
pc	2372.59	kPa	Joback Method
rinpol	1406.40		NIST Webbook
tb	550.95	K	Joback Method
tc	795.54	K	Joback Method
tf	297.60 ± 0.30	K	NIST Webbook
vc	0.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.75	J/mol×K	591.71	Joback Method
cpg	513.58	J/mol×K	632.48	Joback Method
cpg	539.59	J/mol×K	673.24	Joback Method
cpg	606.58	J/mol×K	795.54	Joback Method
cpg	563.77	J/mol×K	714.01	Joback Method
cpg	586.10	J/mol×K	754.77	Joback Method
cpg	456.11	J/mol×K	550.95	Joback Method

dvisc	0.0000734	Pa×s	496.33	Joback Method
dvisc	0.0001712	Pa×s	441.72	Joback Method
dvisc	0.0005072	Pa×s	387.10	Joback Method
dvisc	0.0021468	Pa×s	332.48	Joback Method
dvisc	0.0160230	Pa×s	277.87	Joback Method
dvisc	0.0000372	Pa×s	550.95	Joback Method
dvisc	0.3197583	Pa×s	223.25	Joback Method
hfust	0.90	kJ/mol	285.60	NIST Webbook
hfust	7.40	kJ/mol	297.60	NIST Webbook
hfust	7.40	kJ/mol	297.60	NIST Webbook
sfust	24.87	J/mol×K	297.60	NIST Webbook
sfust	3.15	J/mol×K	285.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43931e+01
Coeff. B	-4.31209e+03
Coeff. C	-8.27900e+01
Temperature range (K), min.	388.49
Temperature range (K), max.	557.60

Sources

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=C295023&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

Legend

chl: Standard liquid 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
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion 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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume