1,8-Cyclotetradecadiyne

Inchi: InChI=1S/C14H20/c1-2-4-6-8-10-12-14-13-11-9-7-5-3-1/h1-5,10-14H2
InchiKey: BVTCHBNCNJEJTD-UHFFFAOYSA-N
Formula: C14H20
SMILES: C1#CCCCCCC#CCCCCC1
Mol. weight [g/mol]: 188.31
CAS: 1540-80-3

Physical Properties

Property code	Value	Unit	Source
chs	-8515.20 ± 1.70	kJ/mol	NIST Webbook
hf	313.80 ± 4.00	kJ/mol	NIST Webbook
hfs	147.70 ± 2.30	kJ/mol	NIST Webbook
hsub	94.30	kJ/mol	NIST Webbook
hsub	166.10	kJ/mol	NIST Webbook
log10ws	-5.17		Crippen Method
logp	3.908		Crippen Method
mcvol	180.060	ml/mol	McGowan Method
tf	370.00 ± 0.30	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	22.60	kJ/mol	370.00	NIST Webbook
hfust	22.60	kJ/mol	370.00	NIST Webbook
hsubt	87.60 ± 1.00	kJ/mol	339.50	NIST Webbook
hsubt	166.00 ± 3.20	kJ/mol	355.00	NIST Webbook
hsubt	166.00 ± 3.20	kJ/mol	324.50	NIST Webbook

Correlations

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	7.79785e+00
Coeff. B	-9.90328e+02
Coeff. C	-2.20016e+02
Temperature range (K), min.	351.88
Temperature range (K), max.	618.32

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1540803&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation 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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
tf:	Normal melting (fusion) point