1-Hydroxy-1-ethynylcyclododecane

Inchi: InChI=1S/C14H24O/c1-2-14(15)12-10-8-6-4-3-5-7-9-11-13-14/h1,15H,3-13H2
InchiKey: DCHDUZYXRMNPCU-UHFFFAOYSA-N
Formula: C14H24O
SMILES: C#CC1(O)CCCCCCCCCCC1
Mol. weight [g/mol]: 208.34

Physical Properties

Property code	Value	Unit	Source
gf	99.61	kJ/mol	Joback Method
hf	-160.02	kJ/mol	Joback Method
hfus	12.02	kJ/mol	Joback Method
hvap	63.61	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	3.655		Crippen Method
mcvol	194.530	ml/mol	McGowan Method
pc	2707.03	kPa	Joback Method
rinpol	1641.00		NIST Webbook
rinpol	1657.90		NIST Webbook
rinpol	1632.20		NIST Webbook
rinpol	1657.90		NIST Webbook
rinpol	1641.00		NIST Webbook
rinpol	1632.20		NIST Webbook
rinpol	1657.90		NIST Webbook
rinpol	1632.20		NIST Webbook
ripol	2318.40		NIST Webbook
ripol	2361.70		NIST Webbook
ripol	2289.70		NIST Webbook
ripol	2361.70		NIST Webbook
ripol	2289.70		NIST Webbook
ripol	2361.70		NIST Webbook
ripol	2289.70		NIST Webbook
ripol	2318.40		NIST Webbook
tb	647.43	K	Joback Method
tc	883.27	K	Joback Method
tf	365.49	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	542.23	J/mol×K	647.43	Joback Method
cpg	565.02	J/mol×K	686.74	Joback Method
cpg	586.41	J/mol×K	726.04	Joback Method
cpg	606.49	J/mol×K	765.35	Joback Method
cpg	625.39	J/mol×K	804.65	Joback Method
cpg	643.22	J/mol×K	843.96	Joback Method
cpg	660.10	J/mol×K	883.27	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R235702&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

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
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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume