Heptane, 1,1'-oxybis-

Other names:	1,1'-oxybisheptane
	1-(Heptyloxy)heptane
	Bis(1-heptyl) ether
	Di-n-heptyl ether
	Diheptyl ether
	Ether, di-n-heptyl
	Ether, diheptyl
	Heptyl ether
	NSC 97274
Inchi:	InChI=1S/C14H30O/c1-3-5-7-9-11-13-15-14-12-10-8-6-4-2/h3-14H2,1-2H3
InchiKey:	UJEGHEMJVNQWOJ-UHFFFAOYSA-N
Formula:	C14H30O
SMILES:	CCCCCCCOCCCCCCC
Mol. weight [g/mol]:	214.39
CAS:	629-64-1

Physical Properties

Property code	Value	Unit	Source
gf	-38.00	kJ/mol	Joback Method
hf	-464.51	kJ/mol	Joback Method
hfus	33.20	kJ/mol	Joback Method
hvap	49.17	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	4.944		Crippen Method
mcvol	213.990	ml/mol	McGowan Method
pc	1503.48	kPa	Joback Method
rinpol	1458.00		NIST Webbook
ripol	1550.00		NIST Webbook
tb	542.14	K	Joback Method
tc	701.88	K	Joback Method
tf	269.77	K	Joback Method
vc	0.838	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	633.50	J/mol×K	701.88	Joback Method
cpg	536.33	J/mol×K	542.14	Joback Method
cpg	554.10	J/mol×K	568.76	Joback Method
cpg	571.22	J/mol×K	595.39	Joback Method
cpg	587.72	J/mol×K	622.01	Joback Method
cpg	603.58	J/mol×K	648.63	Joback Method
cpg	618.84	J/mol×K	675.26	Joback Method
dvisc	0.0001482	Pa×s	542.14	Joback Method
dvisc	0.0038629	Pa×s	269.77	Joback Method
dvisc	0.0015169	Pa×s	315.16	Joback Method
dvisc	0.0007537	Pa×s	360.56	Joback Method
dvisc	0.0004379	Pa×s	405.95	Joback Method
dvisc	0.0002838	Pa×s	451.35	Joback Method
dvisc	0.0001991	Pa×s	496.75	Joback Method
hvapt	63.10	kJ/mol	453.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.61961e+01
Coeff. B	-5.06843e+03
Coeff. C	-8.99220e+01
Temperature range (K), min.	408.52
Temperature range (K), max.	555.57

Sources

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

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1026.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C629641&Units=SI

Legend

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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume