DIOCTADECYL ETHER

Other names:	Octadecyl ether
	dioctadecyl ether
	19-Oxaheptatriacontane
Inchi:	InChI=1S/C36H74O/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-37-36-34-32-3
InchiKey:	HBXWUCXDUUJDRB-UHFFFAOYSA-N
Formula:	C36H74O
SMILES:	CCCCCCCCCCCCCCCCCCOCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	522.99

Physical Properties

Property code	Value	Unit	Source
af	1.4824		Cheméo Relay (1.0)
gf	147.24	kJ/mol	Joback Method
hf	-915.87	kJ/mol	Cheméo Relay (1.0)
hfus	90.18	kJ/mol	Joback Method
hvap	174.19	kJ/mol	Cheméo Relay (1.0)
ie	10.07	eV	Cheméo Relay (1.0)
log10ws	-11.90		Cheméo Relay (1.0)
logp	13.526		Crippen Method
mcvol	523.970	ml/mol	McGowan Method
pc	454.43	kPa	Joback Method
tb	684.42	K	Cheméo Relay (1.0)
tc	856.51	K	Cheméo Relay (1.0)
tf	325.02	K	Cheméo Relay (1.0)
vc	2.072	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1930.04	J/mol×K	1045.50	Joback Method
cpg	1965.61	J/mol×K	1096.16	Joback Method
cpg	1997.93	J/mol×K	1146.83	Joback Method
cpg	2027.29	J/mol×K	1197.49	Joback Method
cpg	2053.98	J/mol×K	1248.16	Joback Method

cpg	2078.27	J/mol×K	1298.82	Joback Method
cpg	2100.44	J/mol×K	1349.48	Joback Method
dvisc	0.0002889	Pa×s	517.71	Joback Method
dvisc	0.0000989	Pa×s	605.68	Joback Method
dvisc	0.0000444	Pa×s	693.64	Joback Method
dvisc	0.0000239	Pa×s	781.61	Joback Method
dvisc	0.0000146	Pa×s	869.57	Joback Method
dvisc	0.0000097	Pa×s	957.53	Joback Method
dvisc	0.0000070	Pa×s	1045.50	Joback Method
hfust	105.86	kJ/mol	335.30	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6297036&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af: Acentric Factor
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
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume