Isopropyl triacontyl ether

Inchi: InChI=1S/C33H68O/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-2
InchiKey: YAMBTAVKEBNPIV-UHFFFAOYSA-N
Formula: C33H68O
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCOC(C)C
Mol. weight [g/mol]: 480.89

Physical Properties

Property code	Value	Unit	Source
gf	119.54	kJ/mol	Joback Method
hf	-861.95	kJ/mol	Joback Method
hfus	78.89	kJ/mol	Joback Method
hvap	91.07	kJ/mol	Joback Method
log10ws	-12.84		Crippen Method
logp	12.354		Crippen Method
mcvol	481.700	ml/mol	McGowan Method
pc	517.70	kPa	Joback Method
rinpol	3311.00		NIST Webbook
rinpol	3311.00		NIST Webbook
tb	976.42	K	Joback Method
tc	1225.28	K	Joback Method
tf	468.90	K	Joback Method
vc	1.895	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1723.20	J/mol×K	976.42	Joback Method
cpg	1854.47	J/mol×K	1183.80	Joback Method
cpg	1832.25	J/mol×K	1142.32	Joback Method
cpg	1808.15	J/mol×K	1100.85	Joback Method
cpg	1782.04	J/mol×K	1059.37	Joback Method
cpg	1753.77	J/mol×K	1017.90	Joback Method
cpg	1874.95	J/mol×K	1225.28	Joback Method
dvisc	0.0000102	Pa×s	976.42	Joback Method

dvisc	0.0000145	Pa×s	891.83	Joback Method
dvisc	0.0000221	Pa×s	807.25	Joback Method
dvisc	0.0000371	Pa×s	722.66	Joback Method
dvisc	0.0000715	Pa×s	638.07	Joback Method
dvisc	0.0001683	Pa×s	553.49	Joback Method
dvisc	0.0005402	Pa×s	468.90	Joback Method

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=U406348&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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