Dotriacontyl isobutyl ether

Inchi: InChI=1S/C36H74O/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: DQHNGEPVMUWTHU-UHFFFAOYSA-N
Formula: C36H74O
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCOCC(C)C
Mol. weight [g/mol]: 522.97

Physical Properties

Property code	Value	Unit	Source
gf	144.80	kJ/mol	Joback Method
hf	-923.87	kJ/mol	Joback Method
hfus	86.66	kJ/mol	Joback Method
hvap	97.75	kJ/mol	Joback Method
log10ws	-13.74		Crippen Method
logp	13.382		Crippen Method
mcvol	523.970	ml/mol	McGowan Method
pc	455.99	kPa	Joback Method
rinpol	3620.00		NIST Webbook
rinpol	3620.00		NIST Webbook
tb	1045.06	K	Joback Method
tc	1343.82	K	Joback Method
tf	502.71	K	Joback Method
vc	2.063	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1930.16	J/mol×K	1045.06	Joback Method
cpg	1965.04	J/mol×K	1094.85	Joback Method
cpg	1996.75	J/mol×K	1144.65	Joback Method
cpg	2025.57	J/mol×K	1194.44	Joback Method
cpg	2051.77	J/mol×K	1244.23	Joback Method
cpg	2075.60	J/mol×K	1294.02	Joback Method
cpg	2097.34	J/mol×K	1343.82	Joback Method
dvisc	0.0003396	Pa×s	502.71	Joback Method

dvisc	0.0001054	Pa×s	593.10	Joback Method
dvisc	0.0000446	Pa×s	683.49	Joback Method
dvisc	0.0000230	Pa×s	773.88	Joback Method
dvisc	0.0000137	Pa×s	864.28	Joback Method
dvisc	0.0000090	Pa×s	954.67	Joback Method
dvisc	0.0000063	Pa×s	1045.06	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=U406336&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