Dotriacontyl isopropyl ether

Inchi: InChI=1S/C35H72O/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: NWEWOIRGJUOVMM-UHFFFAOYSA-N
Formula: C35H72O
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCOC(C)C
Mol. weight [g/mol]: 508.95

Physical Properties

Property code	Value	Unit	Source
gf	136.38	kJ/mol	Joback Method
hf	-903.23	kJ/mol	Joback Method
hfus	84.07	kJ/mol	Joback Method
hvap	95.53	kJ/mol	Joback Method
log10ws	-13.67		Crippen Method
logp	13.134		Crippen Method
mcvol	509.880	ml/mol	McGowan Method
pc	475.27	kPa	Joback Method
rinpol	3508.00		NIST Webbook
rinpol	3508.00		NIST Webbook
tb	1022.18	K	Joback Method
tc	1302.47	K	Joback Method
tf	491.44	K	Joback Method
vc	2.007	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1860.93	J/mol×K	1022.18	Joback Method
cpg	1894.25	J/mol×K	1068.90	Joback Method
cpg	1924.74	J/mol×K	1115.61	Joback Method
cpg	1952.60	J/mol×K	1162.33	Joback Method
cpg	1978.05	J/mol×K	1209.04	Joback Method
cpg	2001.31	J/mol×K	1255.76	Joback Method
cpg	2022.59	J/mol×K	1302.47	Joback Method
dvisc	0.0003970	Pa×s	491.44	Joback Method

dvisc	0.0001234	Pa×s	579.90	Joback Method
dvisc	0.0000522	Pa×s	668.35	Joback Method
dvisc	0.0000270	Pa×s	756.81	Joback Method
dvisc	0.0000161	Pa×s	845.27	Joback Method
dvisc	0.0000105	Pa×s	933.72	Joback Method
dvisc	0.0000074	Pa×s	1022.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406349&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

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