Dotriacontanal, 12-methyl

Inchi: InChI=1S/C33H66O/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-18-21-24-27-30-33(2)31-28-
InchiKey: FUWIDCPSLWQYJR-UHFFFAOYSA-N
Formula: C33H66O
SMILES: CCCCCCCCCCCCCCCCCCCCC(C)CCCCCCCCCC=O
Mol. weight [g/mol]: 478.88

Physical Properties

Property code	Value	Unit	Source
gf	125.02	kJ/mol	Joback Method
hf	-815.31	kJ/mol	Joback Method
hfus	79.99	kJ/mol	Joback Method
hvap	95.38	kJ/mol	Joback Method
log10ws	-12.67		Crippen Method
logp	12.154		Crippen Method
mcvol	477.400	ml/mol	McGowan Method
pc	539.83	kPa	Joback Method
rinpol	3462.00		NIST Webbook
tb	1002.66	K	Joback Method
tc	1261.41	K	Joback Method
tf	488.67	K	Joback Method
vc	1.895	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1715.06	J/mol×K	1002.66	Joback Method
cpg	1744.86	J/mol×K	1045.78	Joback Method
cpg	1772.51	J/mol×K	1088.91	Joback Method
cpg	1798.19	J/mol×K	1132.03	Joback Method
cpg	1822.07	J/mol×K	1175.16	Joback Method
cpg	1844.36	J/mol×K	1218.28	Joback Method
cpg	1865.21	J/mol×K	1261.41	Joback Method
dvisc	0.0006755	Pa×s	488.67	Joback Method
dvisc	0.0002218	Pa×s	574.33	Joback Method

dvisc	0.0000973	Pa×s	660.00	Joback Method
dvisc	0.0000515	Pa×s	745.66	Joback Method
dvisc	0.0000311	Pa×s	831.33	Joback Method
dvisc	0.0000207	Pa×s	917.00	Joback Method
dvisc	0.0000147	Pa×s	1002.66	Joback Method

Sources

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=R528564&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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