Triacontanal, 12-methyl

Inchi: InChI=1S/C31H62O/c1-3-4-5-6-7-8-9-10-11-12-13-14-16-19-22-25-28-31(2)29-26-23-20-
InchiKey: RNMRAWWQHFHBND-UHFFFAOYSA-N
Formula: C31H62O
SMILES: CCCCCCCCCCCCCCCCCCC(C)CCCCCCCCCCC=O
Mol. weight [g/mol]: 450.82

Physical Properties

Property code	Value	Unit	Source
gf	108.18	kJ/mol	Joback Method
hf	-774.03	kJ/mol	Joback Method
hfus	74.81	kJ/mol	Joback Method
hvap	90.93	kJ/mol	Joback Method
log10ws	-11.84		Crippen Method
logp	11.374		Crippen Method
mcvol	449.220	ml/mol	McGowan Method
pc	591.42	kPa	Joback Method
rinpol	3261.00		NIST Webbook
tb	956.90	K	Joback Method
tc	1189.23	K	Joback Method
tf	466.13	K	Joback Method
vc	1.782	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1579.66	J/mol×K	956.90	Joback Method
cpg	1699.62	J/mol×K	1150.51	Joback Method
cpg	1678.72	J/mol×K	1111.78	Joback Method
cpg	1656.40	J/mol×K	1073.06	Joback Method
cpg	1632.53	J/mol×K	1034.34	Joback Method
cpg	1606.99	J/mol×K	995.62	Joback Method
cpg	1719.22	J/mol×K	1189.23	Joback Method
dvisc	0.0000202	Pa×s	956.90	Joback Method
dvisc	0.0000283	Pa×s	875.11	Joback Method

dvisc	0.0000425	Pa×s	793.31	Joback Method
dvisc	0.0000701	Pa×s	711.51	Joback Method
dvisc	0.0001319	Pa×s	629.72	Joback Method
dvisc	0.0002995	Pa×s	547.92	Joback Method
dvisc	0.0009070	Pa×s	466.13	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=R528579&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

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