

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:	RNMRAWWQHFBND-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/molxK	956.90	Joback Method
cpg	1606.99	J/molxK	995.62	Joback Method
cpg	1632.53	J/molxK	1034.34	Joback Method
cpg	1656.40	J/molxK	1073.06	Joback Method
cpg	1678.72	J/molxK	1111.78	Joback Method
cpg	1699.62	J/molxK	1150.51	Joback Method
cpg	1719.22	J/molxK	1189.23	Joback Method
dvisc	0.0009070	Paxs	466.13	Joback Method
dvisc	0.0002995	Paxs	547.92	Joback Method

dvisc	0.0001319	Paxs	629.72	Joback Method
dvisc	0.0000701	Paxs	711.51	Joback Method
dvisc	0.0000425	Paxs	793.31	Joback Method
dvisc	0.0000283	Paxs	875.11	Joback Method
dvisc	0.0000202	Paxs	956.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R528579&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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