

Triacontanal

Inchi:

InChI=1S/C30H60O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24

InchiKey:

CGNVIRPGBUXJES-UHFFFAOYSA-N

Formula:

C30H60O

SMILES:

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC=O

Mol. weight [g/mol]:

436.80

CAS:

22725-63-9

Physical Properties

Property code	Value	Unit	Source
gf	102.20	kJ/mol	Joback Method
hf	-748.11	kJ/mol	Joback Method
hfus	75.75	kJ/mol	Joback Method
hvap	89.09	kJ/mol	Joback Method
log10ws	-11.66		Crippen Method
logp	11.128		Crippen Method
mcvol	435.130	ml/mol	McGowan Method
pc	617.57	kPa	Joback Method
rinpol	3251.20		NIST Webbook
rinpol	3251.20		NIST Webbook
tb	934.46	K	Joback Method
tc	1157.85	K	Joback Method
tf	469.86	K	Joback Method
vc	1.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1512.23	J/mol×K	934.46	Joback Method
cpg	1629.40	J/mol×K	1120.62	Joback Method
cpg	1608.86	J/mol×K	1083.39	Joback Method
cpg	1586.98	J/mol×K	1046.16	Joback Method
cpg	1563.66	J/mol×K	1008.92	Joback Method
cpg	1538.77	J/mol×K	971.69	Joback Method
cpg	1648.70	J/mol×K	1157.85	Joback Method

dvisc	0.0000258	Pa×s	934.46	Joback Method
dvisc	0.0000356	Pa×s	857.03	Joback Method
dvisc	0.0000523	Pa×s	779.59	Joback Method
dvisc	0.0000838	Pa×s	702.16	Joback Method
dvisc	0.0001508	Pa×s	624.73	Joback Method
dvisc	0.0003204	Pa×s	547.29	Joback Method
dvisc	0.0008728	Pa×s	469.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22725639&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
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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