12-Hentriacontanone

Inchi: InChI=1S/C31H62O/c1-3-5-7-9-11-13-14-15-16-17-18-19-20-22-24-26-28-30-31(32)29-2
InchiKey: NMZKKVFRTDBHQF-UHFFFAOYSA-N
Formula: C31H62O
SMILES: CCCCCCCCCCCCCCCCCCCC(=O)CCCCCCCCCC
Mol. weight [g/mol]: 450.82
CAS: 16329-85-4

Physical Properties

Property code	Value	Unit	Source
gf	81.22	kJ/mol	Joback Method
hf	-795.75	kJ/mol	Joback Method
hfus	77.65	kJ/mol	Joback Method
hvap	91.35	kJ/mol	Joback Method
log10ws	-12.08		Crippen Method
logp	11.518		Crippen Method
mcvol	449.220	ml/mol	McGowan Method
pc	585.99	kPa	Joback Method
rinpol	3307.60		NIST Webbook
rinpol	3307.60		NIST Webbook
tb	962.55	K	Joback Method
tc	1197.11	K	Joback Method
tf	489.06	K	Joback Method
vc	1.778	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1581.38	J/mol×K	962.55	Joback Method
cpg	1608.78	J/mol×K	1001.64	Joback Method
cpg	1634.36	J/mol×K	1040.74	Joback Method
cpg	1658.24	J/mol×K	1079.83	Joback Method
cpg	1680.55	J/mol×K	1118.92	Joback Method
cpg	1701.41	J/mol×K	1158.02	Joback Method
cpg	1720.95	J/mol×K	1197.11	Joback Method

dvisc	0.0006463	Pa×s	489.06	Joback Method
dvisc	0.0002408	Pa×s	567.98	Joback Method
dvisc	0.0001141	Pa×s	646.89	Joback Method
dvisc	0.0000636	Pa×s	725.80	Joback Method
dvisc	0.0000398	Pa×s	804.72	Joback Method
dvisc	0.0000271	Pa×s	883.63	Joback Method
dvisc	0.0000196	Pa×s	962.55	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=C16329854&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

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