(Z)-Hentriacont-22-ene-2,4-dione

Inchi: InChI=1S/C31H58O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-2
InchiKey: PCUWNQVNMSDXMY-KHPPLWFESA-N
Formula: C31H58O2
SMILES: CCCCCCCCC=CCCCCCCCCCCCCCCCCCCC(=O)CC(C)=O
Mol. weight [g/mol]: 462.79
CAS: 305805-41-8

Physical Properties

Property code	Value	Unit	Source
gf	32.52	kJ/mol	Joback Method
hf	-791.11	kJ/mol	Joback Method
hfus	79.45	kJ/mol	Joback Method
hvap	98.05	kJ/mol	Joback Method
log10ws	-11.21		Crippen Method
logp	10.473		Crippen Method
mcvol	446.490	ml/mol	McGowan Method
pc	620.03	kPa	Joback Method
rinpol	3426.30		NIST Webbook
rinpol	3426.30		NIST Webbook
tb	1020.58	K	Joback Method
tc	1271.90	K	Joback Method
tf	533.91	K	Joback Method
vc	1.764	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1579.37	J/mol×K	1020.58	Joback Method
cpg	1605.03	J/mol×K	1062.47	Joback Method
cpg	1629.02	J/mol×K	1104.35	Joback Method
cpg	1651.52	J/mol×K	1146.24	Joback Method
cpg	1672.68	J/mol×K	1188.13	Joback Method
cpg	1692.69	J/mol×K	1230.01	Joback Method
cpg	1711.71	J/mol×K	1271.90	Joback Method

dvisc	0.0004371	Pa×s	533.91	Joback Method
dvisc	0.0001753	Pa×s	615.02	Joback Method
dvisc	0.0000870	Pa×s	696.13	Joback Method
dvisc	0.0000500	Pa×s	777.25	Joback Method
dvisc	0.0000319	Pa×s	858.36	Joback Method
dvisc	0.0000220	Pa×s	939.47	Joback Method
dvisc	0.0000161	Pa×s	1020.58	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=C305805418&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