(Z)-Tritriacont-24-ene-2,4-dione

Inchi: InChI=1S/C33H62O2/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: PYQSSJXHPITMSX-KHPPLWFESA-N
Formula: C33H62O2
SMILES: CCCCCCCCC=CCCCCCCCCCCCCCCCCCCCCC(=O)CC(C)=O
Mol. weight [g/mol]: 490.84
CAS: 305805-42-9

Physical Properties

Property code	Value	Unit	Source
gf	49.36	kJ/mol	Joback Method
hf	-832.39	kJ/mol	Joback Method
hfus	84.63	kJ/mol	Joback Method
hvap	102.50	kJ/mol	Joback Method
log10ws	-12.05		Crippen Method
logp	11.253		Crippen Method
mcvol	474.670	ml/mol	McGowan Method
pc	564.74	kPa	Joback Method
rinpol	3651.20		NIST Webbook
rinpol	3651.20		NIST Webbook
tb	1066.34	K	Joback Method
tc	1346.55	K	Joback Method
tf	556.45	K	Joback Method
vc	1.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1713.25	J/mol×K	1066.34	Joback Method
cpg	1741.50	J/mol×K	1113.04	Joback Method
cpg	1767.80	J/mol×K	1159.74	Joback Method
cpg	1792.40	J/mol×K	1206.44	Joback Method
cpg	1815.57	J/mol×K	1253.15	Joback Method
cpg	1837.54	J/mol×K	1299.85	Joback Method
cpg	1858.57	J/mol×K	1346.55	Joback Method

dvisc	0.0003299	Pa×s	556.45	Joback Method
dvisc	0.0001308	Pa×s	641.43	Joback Method
dvisc	0.0000644	Pa×s	726.41	Joback Method
dvisc	0.0000368	Pa×s	811.39	Joback Method
dvisc	0.0000233	Pa×s	896.38	Joback Method
dvisc	0.0000160	Pa×s	981.36	Joback Method
dvisc	0.0000117	Pa×s	1066.34	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=C305805429&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