16E,23E-Tetraconta-dien-3-one

Other names: Tetraconta-16E,23E-dien-3-one
Inchi: InChI=1S/C40H76O/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-2
InchiKey: XMEBNQZQPQPETJ-BLKTUOACSA-N
Formula: C40H76O
SMILES: CCCCCCCCCCCCCCCCC=CCCCCCC=CCCCCCCCCCCCCC(=O)CC
Mol. weight [g/mol]: 573.03

Physical Properties

Property code	Value	Unit	Source
gf	317.44	kJ/mol	Joback Method
hf	-747.07	kJ/mol	Joback Method
hfus	101.36	kJ/mol	Joback Method
hvap	111.30	kJ/mol	Joback Method
log10ws	-15.55		Crippen Method
logp	14.581		Crippen Method
mcvol	567.430	ml/mol	McGowan Method
pc	418.03	kPa	Joback Method
rinpol	4179.00		NIST Webbook
rinpol	4179.00		NIST Webbook
tb	1176.79	K	Joback Method
tc	1569.63	K	Joback Method
tf	580.33	K	Joback Method
vc	2.241	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2146.55	J/mol×K	1176.79	Joback Method
cpg	2190.17	J/mol×K	1242.26	Joback Method
cpg	2231.66	J/mol×K	1307.74	Joback Method
cpg	2271.93	J/mol×K	1373.21	Joback Method
cpg	2311.93	J/mol×K	1438.68	Joback Method
cpg	2352.56	J/mol×K	1504.16	Joback Method
cpg	2394.77	J/mol×K	1569.63	Joback Method

dvisc	0.0001497	Pa×s	580.33	Joback Method
dvisc	0.0000510	Pa×s	679.74	Joback Method
dvisc	0.0000228	Pa×s	779.15	Joback Method
dvisc	0.0000123	Pa×s	878.56	Joback Method
dvisc	0.0000075	Pa×s	977.97	Joback Method
dvisc	0.0000050	Pa×s	1077.38	Joback Method
dvisc	0.0000036	Pa×s	1176.79	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=R407333&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

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