

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

Other names:	Tetraconta-16E,23E-dien-3-one
Inchi:	InChI=1S/C40H76O/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26
InchiKey:	XMEBNQZQPQPETJ-BLKTUOACSA-N
Formula:	C40H76O
SMILES:	CCCCCCCCCCCCCCCCCC=CCCCCCC=CCCCCCCCCCCCCCC(=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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0000036	Paxs	1176.79	Joback Method
dvisc	0.0000050	Paxs	1077.38	Joback Method
dvisc	0.0000075	Paxs	977.97	Joback Method
dvisc	0.0000123	Paxs	878.56	Joback Method
dvisc	0.0000228	Paxs	779.15	Joback Method
dvisc	0.0000510	Paxs	679.74	Joback Method
dvisc	0.0001497	Paxs	580.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R407333&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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