

9E,16E,23E-Tetraconta-trien-3-one

Other names:	Tetraconta-9E,16E,23E-trien-3-one
Inchi:	InChI=1S/C40H74O/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:	GJQPXCXKVSVMJ-BMALKTGUSA-N
Formula:	C40H74O
SMILES:	CCCCCCCCCCCCCCCCCC=CCCCCCC=CCCCCCC=CCCCCCC(=O)CC
Mol. weight [g/mol]:	571.01

Physical Properties

Property code	Value	Unit	Source
gf	397.66	kJ/mol	Joback Method
hf	-629.85	kJ/mol	Joback Method
hfus	101.56	kJ/mol	Joback Method
hvap	111.25	kJ/mol	Joback Method
log10ws	-15.41		Crippen Method
logp	14.357		Crippen Method
mcvol	563.130	ml/mol	McGowan Method
pc	427.06	kPa	Joback Method
rinpol	4165.00		NIST Webbook
rinpol	4165.00		NIST Webbook
rinpol	4165.00		NIST Webbook
tb	1180.95	K	Joback Method
tc	1562.52	K	Joback Method
tf	575.25	K	Joback Method
vc	2.221	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2120.03	J/molxK	1180.95	Joback Method
cpg	2163.93	J/molxK	1244.55	Joback Method
cpg	2206.59	J/molxK	1308.14	Joback Method
cpg	2248.95	J/molxK	1371.74	Joback Method
cpg	2291.92	J/molxK	1435.33	Joback Method
cpg	2336.42	J/molxK	1498.93	Joback Method

cpg	2383.38	J/mol×K	1562.52	Joback Method
dvisc	0.0001402	Paxs	575.25	Joback Method
dvisc	0.0000465	Paxs	676.20	Joback Method
dvisc	0.0000206	Paxs	777.15	Joback Method
dvisc	0.0000110	Paxs	878.10	Joback Method
dvisc	0.0000067	Paxs	979.05	Joback Method
dvisc	0.0000044	Paxs	1080.00	Joback Method
dvisc	0.0000032	Paxs	1180.95	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R407393&Units=SI

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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