

9E,16E,23E,30E-octatriaconta-tetraen-3-one

Other names:	Octatriaconta-9E,16E,23E,30E-tetraen-3-one
Inchi:	InChI=1S/C38H68O/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-27-28-29-30-31-32-33-34-35-36-37-38
InchiKey:	ZUOUHKCYMKZKKW-NWVFWHWQVSA-N
Formula:	C38H68O
SMILES:	CCCCCCCC=CCCCCCC=CCCCCCC=CCCCCCC=CCCCCCC(=O)CC
Mol. weight [g/mol]:	540.95

Physical Properties

Property code	Value	Unit	Source
gf	461.04	kJ/mol	Joback Method
hf	-471.35	kJ/mol	Joback Method
hfus	96.58	kJ/mol	Joback Method
hvap	106.76	kJ/mol	Joback Method
log10ws	-14.42		Crippen Method
logp	13.353		Crippen Method
mcpvol	530.650	ml/mol	McGowan Method
pc	473.62	kPa	Joback Method
rinpol	3958.00		NIST Webbook
rinpol	3958.00		NIST Webbook
rinpol	3958.00		NIST Webbook
tb	1139.35	K	Joback Method
tc	1464.61	K	Joback Method
tf	547.63	K	Joback Method
vc	2.090	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1951.52	J/molxK	1139.35	Joback Method
cpg	2138.75	J/molxK	1410.40	Joback Method
cpg	2100.51	J/molxK	1356.19	Joback Method
cpg	2063.26	J/molxK	1301.98	Joback Method
cpg	2026.40	J/molxK	1247.77	Joback Method
cpg	1989.35	J/molxK	1193.56	Joback Method

cpg	2178.59	J/molxK	1464.61	Joback Method
dvisc	0.0000039	Paxs	1139.35	Joback Method
dvisc	0.0000054	Paxs	1040.73	Joback Method
dvisc	0.0000081	Paxs	942.11	Joback Method
dvisc	0.0000135	Paxs	843.49	Joback Method
dvisc	0.0000254	Paxs	744.87	Joback Method
dvisc	0.0000580	Paxs	646.25	Joback Method
dvisc	0.0001788	Paxs	547.63	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=R407373&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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

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