

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

Other names:	9E,16E,23E-octatriaconta-trien-3-one
Inchi:	InChI=1S/C38H70O/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:	ZCSIKXHAMSQWSS-FMFOQKLUSA-N
Formula:	C38H70O
SMILES:	CCCCCCCCCCCCCCCC=CCCCCCC=CCCCCCC=CCCCCCC(=O)CC
Mol. weight [g/mol]:	542.96

Physical Properties

Property code	Value	Unit	Source
gf	380.82	kJ/mol	Joback Method
hf	-588.57	kJ/mol	Joback Method
hfus	96.38	kJ/mol	Joback Method
hvap	106.80	kJ/mol	Joback Method
log10ws	-14.57		Crippen Method
logp	13.577		Crippen Method
mvol	534.950	ml/mol	McGowan Method
pc	463.08	kPa	Joback Method
rinpol	3973.00		NIST Webbook
rinpol	3973.00		NIST Webbook
tb	1135.19	K	Joback Method
tc	1468.47	K	Joback Method
tf	552.71	K	Joback Method
vc	2.110	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1978.69	J/molxK	1135.19	Joback Method
cpg	2016.57	J/molxK	1190.74	Joback Method
cpg	2053.05	J/molxK	1246.28	Joback Method
cpg	2088.74	J/molxK	1301.83	Joback Method
cpg	2124.22	J/molxK	1357.38	Joback Method
cpg	2160.08	J/molxK	1412.93	Joback Method
cpg	2196.92	J/molxK	1468.47	Joback Method

dvisc	0.0001908	Paxs	552.71	Joback Method
dvisc	0.0000636	Paxs	649.79	Joback Method
dvisc	0.0000282	Paxs	746.87	Joback Method
dvisc	0.0000151	Paxs	843.95	Joback Method
dvisc	0.0000092	Paxs	941.03	Joback Method
dvisc	0.0000061	Paxs	1038.11	Joback Method
dvisc	0.0000044	Paxs	1135.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R407388&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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