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

Other names: 9E,16E,23E-octatriaconta-trien-3-one
Inchi: InChI=1S/C38H70O/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-2
InchiKey: ZCSIKXHAMSQWSS-FMFOQKLUSA-N
Formula: C38H70O
SMILES: CCCCCCCCCCCCCCC=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
mcvol	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	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0000044	Pa×s	1135.19	Joback Method
dvisc	0.0000061	Pa×s	1038.11	Joback Method
dvisc	0.0000092	Pa×s	941.03	Joback Method
dvisc	0.0000151	Pa×s	843.95	Joback Method
dvisc	0.0000282	Pa×s	746.87	Joback Method
dvisc	0.0000636	Pa×s	649.79	Joback Method
dvisc	0.0001908	Pa×s	552.71	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=R407388&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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

Latest version available from:
https://www.chemeo.com/cid/16-252-4/Octatriaconta-9E-16E-23E-trien-3-one.pdf
Generated by Cheméo on 2024-10-12 02:35:52.528268496 +0000 UTC m=+3281415.165237744.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.