

8E,15E,22E-nonatriaconta-trien-2-one

Other names:	Nonatriaconta-8E,15E,22E-trien-2-one
Inchi:	InChI=1S/C39H72O/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25
InchiKey:	SLHWPHNHPLMDPP-VUGIOZIKSA-N
Formula:	C39H72O
SMILES:	CCCCCCCCCCCCCCCCCC=CCCCCCC=CCCCCCC=CCCCCCC(C)=O
Mol. weight [g/mol]:	556.99

Physical Properties

Property code	Value	Unit	Source
gf	389.24	kJ/mol	Joback Method
hf	-609.21	kJ/mol	Joback Method
hfus	98.97	kJ/mol	Joback Method
hvap	109.03	kJ/mol	Joback Method
log10ws	-14.99		Crippen Method
logp	13.967		Crippen Method
mcvol	549.040	ml/mol	McGowan Method
pc	444.52	kPa	Joback Method
rinpol	4073.00		NIST Webbook
rinpol	4073.00		NIST Webbook
tb	1158.07	K	Joback Method
tc	1514.26	K	Joback Method
tf	563.98	K	Joback Method
vc	2.166	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2049.13	J/molxK	1158.07	Joback Method
cpg	2089.83	J/molxK	1217.43	Joback Method
cpg	2129.19	J/molxK	1276.80	Joback Method
cpg	2167.95	J/molxK	1336.16	Joback Method
cpg	2206.84	J/molxK	1395.53	Joback Method
cpg	2246.60	J/molxK	1454.89	Joback Method
cpg	2287.96	J/molxK	1514.26	Joback Method

dvisc	0.0001637	Paxs	563.98	Joback Method
dvisc	0.0000544	Paxs	663.00	Joback Method
dvisc	0.0000241	Paxs	762.01	Joback Method
dvisc	0.0000129	Paxs	861.02	Joback Method
dvisc	0.0000078	Paxs	960.04	Joback Method
dvisc	0.0000052	Paxs	1059.05	Joback Method
dvisc	0.0000037	Paxs	1158.07	Joback Method

Sources

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=R407368&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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