

15E,22E-nonatriaconta-dien-2-one

Other names:	Nonatriaconta-15E,22E-dien-2-one
Inchi:	InChI=1S/C39H74O/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:	MHNHPKZTUVMCRT-NJGOVPIFSA-N
Formula:	C39H74O
SMILES:	CCCCCCCCCCCCCCCCCC=CCCCCCC=CCCCCCCCCCCCCCC(C)=O
Mol. weight [g/mol]:	559.00

Physical Properties

Property code	Value	Unit	Source
gf	309.02	kJ/mol	Joback Method
hf	-726.43	kJ/mol	Joback Method
hfus	98.77	kJ/mol	Joback Method
hvap	109.07	kJ/mol	Joback Method
log10ws	-15.14		Crippen Method
logp	14.191		Crippen Method
mcvol	553.340	ml/mol	McGowan Method
pc	434.93	kPa	Joback Method
rinpol	4087.00		NIST Webbook
rinpol	4087.00		NIST Webbook
rinpol	4087.00		NIST Webbook
tb	1153.91	K	Joback Method
tc	1519.99	K	Joback Method
tf	569.06	K	Joback Method
vc	2.186	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2076.07	J/molxK	1153.91	Joback Method
cpg	2116.72	J/molxK	1214.92	Joback Method
cpg	2155.26	J/molxK	1275.94	Joback Method
cpg	2192.42	J/molxK	1336.95	Joback Method
cpg	2228.94	J/molxK	1397.96	Joback Method
cpg	2265.55	J/molxK	1458.97	Joback Method

cpg	2302.99	J/mol×K	1519.99	Joback Method
dvisc	0.0001748	Paxs	569.06	Joback Method
dvisc	0.0000597	Paxs	666.53	Joback Method
dvisc	0.0000268	Paxs	764.01	Joback Method
dvisc	0.0000144	Paxs	861.48	Joback Method
dvisc	0.0000088	Paxs	958.96	Joback Method
dvisc	0.0000059	Paxs	1056.43	Joback Method
dvisc	0.0000042	Paxs	1153.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R407313&Units=SI
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

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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