

16E,23E-octatriaconta-dien-3-one

Other names:	Octatriaconta-16E,23E-dien-3-one
Inchi:	InChI=1S/C38H72O/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:	LSJKYNABDLNZPV-YRVRKSHPSA-N
Formula:	C38H72O
SMILES:	CCCCCCCCCCCCCCCC=CCCCCCC=CCCCCCCCCCCCCCCC(=O)CC
Mol. weight [g/mol]:	544.98

Physical Properties

Property code	Value	Unit	Source
gf	300.60	kJ/mol	Joback Method
hf	-705.79	kJ/mol	Joback Method
hfus	96.18	kJ/mol	Joback Method
hvap	106.84	kJ/mol	Joback Method
log10ws	-14.72		Crippen Method
logp	13.801		Crippen Method
mvol	539.250	ml/mol	McGowan Method
pc	452.89	kPa	Joback Method
rinpol	3986.00		NIST Webbook
rinpol	3986.00		NIST Webbook
tb	1131.03	K	Joback Method
tc	1472.93	K	Joback Method
tf	557.79	K	Joback Method
vc	2.130	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2005.96	J/mol×K	1131.03	Joback Method
cpg	2043.96	J/mol×K	1188.01	Joback Method
cpg	2079.92	J/mol×K	1245.00	Joback Method
cpg	2114.42	J/mol×K	1301.98	Joback Method
cpg	2148.04	J/mol×K	1358.96	Joback Method
cpg	2181.37	J/mol×K	1415.95	Joback Method
cpg	2215.00	J/mol×K	1472.93	Joback Method

dvisc	0.0002037	Paxs	557.79	Joback Method
dvisc	0.0000698	Paxs	653.33	Joback Method
dvisc	0.0000314	Paxs	748.87	Joback Method
dvisc	0.0000169	Paxs	844.41	Joback Method
dvisc	0.0000104	Paxs	939.95	Joback Method
dvisc	0.0000069	Paxs	1035.49	Joback Method
dvisc	0.0000050	Paxs	1131.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R407328&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
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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