

9,12,15-Octadecatrien-1-ol, (Z,Z,Z)-

Other names:	(Z,Z,Z)-9,12,15-Octadecatrien-1-ol (9Z,12Z,15Z)-9,12,15-octadecatrien-1-ol
Inchi:	InChI=1S/C18H32O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19/h3-4,6-7,9-10,19
InchiKey:	IKYKEVDKGZYRMQ-IUQGGRGSQSA-N
Formula:	C18H32O
SMILES:	CCC=CCC=CCC=CCCCCCCCCO
Mol. weight [g/mol]:	264.45
CAS:	506-44-5

Physical Properties

Property code	Value	Unit	Source
gf	204.52	kJ/mol	Joback Method
hf	-215.42	kJ/mol	Joback Method
hfus	47.07	kJ/mol	Joback Method
hvap	72.22	kJ/mol	Joback Method
log10ws	-6.18		Crippen Method
logp	5.568		Crippen Method
mcvol	257.450	ml/mol	McGowan Method
pc	1373.78	kPa	Joback Method
rinpol	2057.50		NIST Webbook
rinpol	2058.00		NIST Webbook
rinpol	2058.00		NIST Webbook
rinpol	2058.00		NIST Webbook
rinpol	2057.50		NIST Webbook
tb	715.90	K	Joback Method
tc	889.40	K	Joback Method
tf	338.20	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.66	J/molxK	715.90	Joback Method
cpg	756.11	J/molxK	744.82	Joback Method

cpg	771.81	J/molxK	773.73	Joback Method
cpg	786.83	J/molxK	802.65	Joback Method
cpg	801.20	J/molxK	831.57	Joback Method
cpg	814.99	J/molxK	860.48	Joback Method
cpg	828.24	J/molxK	889.40	Joback Method
dvisc	0.0053100	Paxs	338.20	Joback Method
dvisc	0.0009746	Paxs	401.15	Joback Method
dvisc	0.0002833	Paxs	464.10	Joback Method
dvisc	0.0001107	Paxs	527.05	Joback Method
dvisc	0.0000528	Paxs	590.00	Joback Method
dvisc	0.0000291	Paxs	652.95	Joback Method
dvisc	0.0000178	Paxs	715.90	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C506445&Units=SI

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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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