E,Z-2,13-OCTADECADIEN-1-OL

Other names: (E,Z)-2,13-octadecadienol
(E)-2-(Z)-13-Octadecadien-1-ol
Inchi: InChI=1S/C18H34O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19/h5-6,16-17,19H,
InchiKey: YCOMGIOWVNOOBC-RAPDCGKPSA-N
Formula: C18H34O
SMILES: CCCC/C=C\CCCCCCCCC/C=C/CO
Mol. weight [g/mol]: 266.47

Physical Properties

Property code	Value	Unit	Source
af	0.8943		Cheméo Relay (1.0)
gf	124.30	kJ/mol	Joback Method
hf	-424.38	kJ/mol	Cheméo Relay (1.0)
hfus	46.87	kJ/mol	Joback Method
hvap	118.99	kJ/mol	Cheméo Relay (1.0)
ie	8.73	eV	Cheméo Relay (1.0)
log10ws	-6.26		Cheméo Relay (1.0)
logp	5.792		Crippen Method
mcvol	261.750	ml/mol	McGowan Method
pc	1322.31	kPa	Joback Method
rinpol	2076.00		NIST Webbook
rinpol	2075.00		NIST Webbook
ripol	2191.00		NIST Webbook
tb	595.48	K	Cheméo Relay (1.0)
tc	786.44	K	Cheméo Relay (1.0)
tf	289.64	K	Cheméo Relay (1.0)
vc	0.949	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.54	J/mol×K	711.74	Joback Method
cpg	779.51	J/mol×K	740.04	Joback Method
cpg	795.72	J/mol×K	768.33	Joback Method

cpg	811.22	J/mol×K	796.63	Joback Method
cpg	826.06	J/mol×K	824.93	Joback Method
cpg	840.26	J/mol×K	853.23	Joback Method
cpg	853.88	J/mol×K	881.52	Joback Method
dvisc	0.0053256	Pa×s	343.28	Joback Method
dvisc	0.0010481	Pa×s	404.69	Joback Method
dvisc	0.0003165	Pa×s	466.10	Joback Method
dvisc	0.0001263	Pa×s	527.51	Joback Method
dvisc	0.0000611	Pa×s	588.92	Joback Method
dvisc	0.0000339	Pa×s	650.33	Joback Method
dvisc	0.0000208	Pa×s	711.74	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U131100&Units=SI

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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
ripol:	Polar retention indices

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume