Z-2-OCTADECEN-1-OL

Inchi: InChI=1S/C18H36O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19/h16-17,19H,2-15
InchiKey: NMNAESABLXLQEY-MSUUIHNZSA-N
Formula: C18H36O
SMILES: CCCCCCCCCCCCCCCC/C=C\CO
Mol. weight [g/mol]: 268.48

Physical Properties

Property code	Value	Unit	Source
af	0.9804		Cheméo Relay (1.0)
gf	44.08	kJ/mol	Joback Method
hf	-485.44	kJ/mol	Cheméo Relay (1.0)
hfus	46.67	kJ/mol	Joback Method
hvap	117.83	kJ/mol	Cheméo Relay (1.0)
ie	9.26	eV	Cheméo Relay (1.0)
log10ws	-6.64		Cheméo Relay (1.0)
logp	6.016		Crippen Method
mcvol	266.050	ml/mol	McGowan Method
pc	1273.69	kPa	Joback Method
rinpol	2086.00		NIST Webbook
ripol	2145.00		NIST Webbook
ripol	2145.00		NIST Webbook
tb	598.43	K	Cheméo Relay (1.0)
tc	786.30	K	Cheméo Relay (1.0)
tf	312.94	K	Cheméo Relay (1.0)
vc	1.008	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	785.17	J/mol×K	707.58	Joback Method
cpg	802.67	J/mol×K	735.32	Joback Method
cpg	819.41	J/mol×K	763.06	Joback Method
cpg	835.41	J/mol×K	790.79	Joback Method
cpg	850.72	J/mol×K	818.53	Joback Method

cpg	865.37	J/mol×K	846.27	Joback Method
cpg	879.39	J/mol×K	874.01	Joback Method
dvisc	0.0053551	Pa×s	348.36	Joback Method
dvisc	0.0011274	Pa×s	408.23	Joback Method
dvisc	0.0003536	Pa×s	468.10	Joback Method
dvisc	0.0001442	Pa×s	527.97	Joback Method
dvisc	0.0000706	Pa×s	587.84	Joback Method
dvisc	0.0000395	Pa×s	647.71	Joback Method
dvisc	0.0000243	Pa×s	707.58	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U131110&Units=SI
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):

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