

(E)13-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/h5-6,19H,2-4,7-
InchiKey:	XHJRPRSNHKNGLW-AATRIKPKSA-N
Formula:	C18H36O
SMILES:	CCCC=CCCCCCCCCCCCCO
Mol. weight [g/mol]:	268.48

Physical Properties

Property code	Value	Unit	Source
gf	44.08	kJ/mol	Joback Method
hf	-449.86	kJ/mol	Joback Method
hfus	46.67	kJ/mol	Joback Method
hvap	72.30	kJ/mol	Joback Method
log10ws	-6.47		Crippen Method
logp	6.016		Crippen Method
mcvol	266.050	ml/mol	McGowan Method
pc	1273.69	kPa	Joback Method
rinpol	2076.00		NIST Webbook
rinpol	2076.00		NIST Webbook
ripol	2125.00		NIST Webbook
ripol	2125.00		NIST Webbook
tb	707.58	K	Joback Method
tc	874.01	K	Joback Method
tf	348.36	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	785.17	J/molxK	707.58	Joback Method
cpg	865.37	J/molxK	846.27	Joback Method
cpg	850.72	J/molxK	818.53	Joback Method
cpg	835.41	J/molxK	790.79	Joback Method
cpg	819.41	J/molxK	763.06	Joback Method
cpg	802.67	J/molxK	735.32	Joback Method

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

Sources

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=R77785&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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