

(E)-15-Octadecen-1-ol

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C18H36O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19/h4-5,19H,2-3,6-10

FITDPOAZLCWDRO-SNAWJCMRSA-N

C18H36O

CCCC=CCCCCCCCCCCCCO

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	2081.00		NIST Webbook
ripol	2134.00		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/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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R571672&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
mccvol:	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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