3-DECANOL, 6-ETHYL-

Inchi: InChI=1S/C12H26O/c1-4-7-8-11(5-2)9-10-12(13)6-3/h11-13H,4-10H2,1-3H3
InchiKey: ZFVYZHDDIOBINE-UHFFFAOYSA-N
Formula: C12H26O
SMILES: CCCCC(CC)CCC(O)CC
Mol. weight [g/mol]: 186.34

Physical Properties

Property code	Value	Unit	Source
af	0.7067		Cheméo Relay (1.0)
hf	-473.54	kJ/mol	Cheméo Relay (1.0)
hfus	23.88	kJ/mol	Joback Method
hvap	82.03	kJ/mol	Cheméo Relay (1.0)
ie	9.59	eV	Cheméo Relay (1.0)
log10ws	-3.82		Cheméo Relay (1.0)
logp	3.754		Crippen Method
mcvol	185.810	ml/mol	McGowan Method
pc	1954.41	kPa	Joback Method
tb	498.15 ± 4.00	K	NIST Webbook
tc	686.69	K	Cheméo Relay (1.0)
tf	243.81	K	Cheméo Relay (1.0)
vc	0.682	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.00	J/mol×K	565.26	Joback Method
cpg	494.19	J/mol×K	592.39	Joback Method
cpg	508.77	J/mol×K	619.52	Joback Method
cpg	522.76	J/mol×K	646.65	Joback Method
cpg	536.16	J/mol×K	673.79	Joback Method
cpg	549.01	J/mol×K	700.92	Joback Method
cpg	561.31	J/mol×K	728.05	Joback Method
dvisc	0.0773422	Pa×s	255.82	Joback Method
dvisc	0.0092648	Pa×s	307.39	Joback Method

dvisc	0.0020420	Pa×s	358.97	Joback Method
dvisc	0.0006581	Pa×s	410.54	Joback Method
dvisc	0.0002731	Pa×s	462.11	Joback Method
dvisc	0.0001352	Pa×s	513.69	Joback Method
dvisc	0.0000761	Pa×s	565.26	Joback Method

Sources

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=C19780315&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume