

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]:	186.33
CAS:	19780-31-5

Physical Properties

Property code	Value	Unit	Source
gf	-91.54	kJ/mol	Joback Method
hf	-453.80	kJ/mol	Joback Method
hfus	23.88	kJ/mol	Joback Method
hvap	58.21	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
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	728.05	K	Joback Method
tf	255.82	K	Joback Method
vc	0.715	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0020420	Paxs	358.97	Joback Method
dvisc	0.0006581	Paxs	410.54	Joback Method
dvisc	0.0002731	Paxs	462.11	Joback Method
dvisc	0.0001352	Paxs	513.69	Joback Method
dvisc	0.0000761	Paxs	565.26	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=C19780315&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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