

1-Hexanol, 2-ethyl-2-propyl-

Other names:	2-Ethyl-2-propyl-1-hexanol
Inchi:	InChI=1S/C11H24O/c1-4-7-9-11(6-3,10-12)8-5-2/h12H,4-10H2,1-3H3
InchiKey:	GPMZMENG TUFHPF-UHFFFAOYSA-N
Formula:	C11H24O
SMILES:	CCCCC(CC)(CO)CCC
Mol. weight [g/mol]:	172.31
CAS:	54461-00-6

Physical Properties

Property code	Value	Unit	Source
gf	-92.24	kJ/mol	Joback Method
hf	-431.35	kJ/mol	Joback Method
hfus	20.92	kJ/mol	Joback Method
hvap	55.46	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	3.365		Crippen Method
mcvol	171.720	ml/mol	McGowan Method
pc	2137.41	kPa	Joback Method
tb	540.03	K	Joback Method
tc	705.71	K	Joback Method
tf	276.97	K	Joback Method
vc	0.659	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.60	J/molxK	540.03	Joback Method
cpg	498.91	J/molxK	678.09	Joback Method
cpg	486.67	J/molxK	650.48	Joback Method
cpg	473.84	J/molxK	622.87	Joback Method
cpg	460.40	J/molxK	595.26	Joback Method
cpg	446.33	J/molxK	567.64	Joback Method
cpg	510.59	J/molxK	705.71	Joback Method
dvisc	0.0000980	Paxs	540.03	Joback Method

dvisc	0.0001684	Paxs	496.19	Joback Method
dvisc	0.0003212	Paxs	452.34	Joback Method
dvisc	0.0007039	Paxs	408.50	Joback Method
dvisc	0.0018627	Paxs	364.66	Joback Method
dvisc	0.0064311	Paxs	320.81	Joback Method
dvisc	0.0328701	Paxs	276.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54461006&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
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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