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: GPMZMENGTUFHPF-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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.60	J/mol×K	540.03	Joback Method
cpg	446.33	J/mol×K	567.64	Joback Method
cpg	460.40	J/mol×K	595.26	Joback Method
cpg	473.84	J/mol×K	622.87	Joback Method
cpg	486.67	J/mol×K	650.48	Joback Method
cpg	498.91	J/mol×K	678.09	Joback Method
cpg	510.59	J/mol×K	705.71	Joback Method
dvisc	0.0328701	Pa×s	276.97	Joback Method

dvisc	0.0064311	Pa×s	320.81	Joback Method
dvisc	0.0018627	Pa×s	364.66	Joback Method
dvisc	0.0007039	Pa×s	408.50	Joback Method
dvisc	0.0003212	Pa×s	452.34	Joback Method
dvisc	0.0001684	Pa×s	496.19	Joback Method
dvisc	0.0000980	Pa×s	540.03	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C54461006&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Latest version available from:
https://www.chemeo.com/cid/73-151-3/1-Hexanol-2-ethyl-2-propyl.pdf
Generated by Cheméo on 2024-06-15 05:17:12.418935662 +0000 UTC m=+20717881.339512977.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.