

3-ETHYL-4-METHYL-3-HEPTANOL

Other names:	3-heptanol, 3-ethyl-4-methyl-
Inchi:	InChI=1S/C10H22O/c1-5-8-9(4)10(11,6-2)7-3/h9,11H,5-8H2,1-4H3
InchiKey:	CSJYKKPUUXXHEG-UHFFFAOYSA-N
Formula:	C10H22O
SMILES:	CCCC(C)C(O)(CC)CC
Mol. weight [g/mol]:	158.29

Physical Properties

Property code	Value	Unit	Source
af	0.6062		Cheméo Relay (1.0)
gf	-103.10	kJ/mol	Joback Method
hf	-409.77	kJ/mol	Cheméo Relay (1.0)
hfus	14.81	kJ/mol	Joback Method
hvap	63.42	kJ/mol	Cheméo Relay (1.0)
ie	9.17	eV	Cheméo Relay (1.0)
log10ws	-2.21		Cheméo Relay (1.0)
logp	2.974		Crippen Method
mcvol	157.630	ml/mol	McGowan Method
pc	2358.78	kPa	Joback Method
tb	459.94	K	Cheméo Relay (1.0)
tc	652.42	K	Cheméo Relay (1.0)
tf	252.06	K	Cheméo Relay (1.0)
vc	0.548	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.78	J/mol×K	516.71	Joback Method
cpg	398.19	J/mol×K	545.01	Joback Method
cpg	411.92	J/mol×K	573.32	Joback Method
cpg	425.02	J/mol×K	601.62	Joback Method
cpg	437.50	J/mol×K	629.92	Joback Method
cpg	449.39	J/mol×K	658.22	Joback Method
cpg	460.72	J/mol×K	686.53	Joback Method

dvisc	0.0899105	Pa×s	250.70	Joback Method
dvisc	0.0128169	Pa×s	295.03	Joback Method
dvisc	0.0030395	Pa×s	339.37	Joback Method
dvisc	0.0010052	Pa×s	383.71	Joback Method
dvisc	0.0004181	Pa×s	428.04	Joback Method
dvisc	0.0002050	Pa×s	472.38	Joback Method
dvisc	0.0001136	Pa×s	516.71	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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=C66719399&Units=SI

Legend

af:	Acentric Factor
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
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

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