

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]:	158.28
CAS:	66719-39-9

Physical Properties

Property code	Value	Unit	Source
gf	-103.10	kJ/mol	Joback Method
hf	-415.99	kJ/mol	Joback Method
hfus	14.81	kJ/mol	Joback Method
hvap	52.85	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	2.974		Crippen Method
mcvol	157.630	ml/mol	McGowan Method
pc	2358.78	kPa	Joback Method
tb	516.71	K	Joback Method
tc	686.53	K	Joback Method
tf	250.70	K	Joback Method
vc	0.598	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.78	J/molxK	516.71	Joback Method
cpg	398.19	J/molxK	545.01	Joback Method
cpg	411.92	J/molxK	573.32	Joback Method
cpg	425.02	J/molxK	601.62	Joback Method
cpg	437.50	J/molxK	629.92	Joback Method
cpg	449.39	J/molxK	658.22	Joback Method
cpg	460.72	J/molxK	686.53	Joback Method
dvisc	0.0899105	Paxs	250.70	Joback Method

dvisc	0.0128169	Paxs	295.03	Joback Method
dvisc	0.0030395	Paxs	339.37	Joback Method
dvisc	0.0010052	Paxs	383.71	Joback Method
dvisc	0.0004181	Paxs	428.04	Joback Method
dvisc	0.0002050	Paxs	472.38	Joback Method
dvisc	0.0001136	Paxs	516.71	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=C66719399&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	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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