3-Ethyl-4-heptanol

Other names: 3-Ethyl-4-heptanol
Inchi: InChI=1S/C9H20O/c1-4-7-9(10)8(5-2)6-3/h8-10H,4-7H2,1-3H3
InchiKey: TVEJPDXJKNOLDQ-UHFFFAOYSA-N
Formula: C9H20O
SMILES: CCCC(O)C(CC)CC
Mol. weight [g/mol]: 144.26

Physical Properties

Property code	Value	Unit	Source
af	0.6028		Cheméo Relay (1.0)
gf	-116.80	kJ/mol	Joback Method
hf	-392.90	kJ/mol	Cheméo Relay (1.0)
hfus	16.11	kJ/mol	Joback Method
hvap	64.52	kJ/mol	Cheméo Relay (1.0)
ie	9.48	eV	Cheméo Relay (1.0)
log10ws	-2.22		Cheméo Relay (1.0)
logp	2.584		Crippen Method
mcvol	143.540	ml/mol	McGowan Method
pc	2566.29	kPa	Joback Method
tb	456.02	K	Cheméo Relay (1.0)
tc	634.33	K	Cheméo Relay (1.0)
tf	230.84	K	Cheméo Relay (1.0)
vc	0.512	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.77	J/mol×K	496.62	Joback Method
cpg	347.81	J/mol×K	524.15	Joback Method
cpg	360.33	J/mol×K	551.68	Joback Method
cpg	372.35	J/mol×K	579.21	Joback Method
cpg	383.89	J/mol×K	606.75	Joback Method
cpg	394.96	J/mol×K	634.28	Joback Method
cpg	405.56	J/mol×K	661.81	Joback Method

dvisc	0.2091511	Pa×s	222.01	Joback Method
dvisc	0.0215322	Pa×s	267.78	Joback Method
dvisc	0.0043049	Pa×s	313.55	Joback Method
dvisc	0.0012970	Pa×s	359.31	Joback Method
dvisc	0.0005125	Pa×s	405.08	Joback Method
dvisc	0.0002445	Pa×s	450.85	Joback Method
dvisc	0.0001337	Pa×s	496.62	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=C19780428&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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