3-OCTANOL, 3-ETHYL-

Other names: 3-ethyloctan-3-ol
Inchi: InChI=1S/C10H22O/c1-4-7-8-9-10(11,5-2)6-3/h11H,4-9H2,1-3H3
InchiKey: NPQPNSNHYJTUSA-UHFFFAOYSA-N
Formula: C10H22O
SMILES: CCCCCC(O)(CC)CC
Mol. weight [g/mol]: 158.29

Physical Properties

Property code	Value	Unit	Source
af	0.6622		Cheméo Relay (1.0)
gf	-100.66	kJ/mol	Joback Method
hf	-421.19	kJ/mol	Cheméo Relay (1.0)
hfus	18.33	kJ/mol	Joback Method
hvap	65.94	kJ/mol	Cheméo Relay (1.0)
ie	9.34	eV	Cheméo Relay (1.0)
log10ws	-2.46		Cheméo Relay (1.0)
logp	3.118		Crippen Method
mcvol	157.630	ml/mol	McGowan Method
pc	2340.56	kPa	Joback Method
tb	472.15 ± 4.00	K	NIST Webbook
tc	656.34	K	Cheméo Relay (1.0)
tf	261.95	K	Cheméo Relay (1.0)
vc	0.575	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.55	J/mol×K	517.15	Joback Method
cpg	397.63	J/mol×K	544.92	Joback Method
cpg	411.07	J/mol×K	572.70	Joback Method
cpg	423.89	J/mol×K	600.47	Joback Method
cpg	436.13	J/mol×K	628.25	Joback Method
cpg	447.81	J/mol×K	656.02	Joback Method
cpg	458.94	J/mol×K	683.80	Joback Method

dvisc	0.0428890	Pa×s	265.70	Joback Method
dvisc	0.0082611	Pa×s	307.61	Joback Method
dvisc	0.0023619	Pa×s	349.52	Joback Method
dvisc	0.0008829	Pa×s	391.42	Joback Method
dvisc	0.0003993	Pa×s	433.33	Joback Method
dvisc	0.0002077	Pa×s	475.24	Joback Method
dvisc	0.0001201	Pa×s	517.15	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2051323&Units=SI

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):

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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