

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:	NPQPNSNHJTUSA-UHFFFAOYSA-N
Formula:	C10H22O
SMILES:	CCCCC(O)(CC)CC
Mol. weight [g/mol]:	158.28
CAS:	2051-32-3

Physical Properties

Property code	Value	Unit	Source
gf	-100.66	kJ/mol	Joback Method
hf	-410.71	kJ/mol	Joback Method
hfus	18.33	kJ/mol	Joback Method
hvap	53.24	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
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	683.80	K	Joback Method
tf	265.70	K	Joback Method
vc	0.604	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.55	J/mol×K	517.15	Joback Method
cpg	447.81	J/mol×K	656.02	Joback Method
cpg	436.13	J/mol×K	628.25	Joback Method
cpg	423.89	J/mol×K	600.47	Joback Method
cpg	411.07	J/mol×K	572.70	Joback Method
cpg	397.63	J/mol×K	544.92	Joback Method
cpg	458.94	J/mol×K	683.80	Joback Method
dvisc	0.0001201	Paxs	517.15	Joback Method

dvisc	0.0002077	Paxs	475.24	Joback Method
dvisc	0.0003993	Paxs	433.33	Joback Method
dvisc	0.0008829	Paxs	391.43	Joback Method
dvisc	0.0023619	Paxs	349.52	Joback Method
dvisc	0.0082611	Paxs	307.61	Joback Method
dvisc	0.0428890	Paxs	265.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2051323&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

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