

3-Octanol, 6-ethyl-

Other names:	6-Ethyl-3-octanol
Inchi:	InChI=1S/C10H22O/c1-4-9(5-2)7-8-10(11)6-3/h9-11H,4-8H2,1-3H3
InchiKey:	JWZFCOOWAQHCBP-UHFFFAOYSA-N
Formula:	C10H22O
SMILES:	CCC(O)CCC(CC)CC
Mol. weight [g/mol]:	158.28
CAS:	19781-27-2

Physical Properties

Property code	Value	Unit	Source
gf	-108.38	kJ/mol	Joback Method
hf	-412.52	kJ/mol	Joback Method
hfus	18.70	kJ/mol	Joback Method
hvap	53.76	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	2.974		Crippen Method
mcvol	157.630	ml/mol	McGowan Method
pc	2333.78	kPa	Joback Method
tb	519.50	K	Joback Method
tc	683.75	K	Joback Method
tf	233.28	K	Joback Method
vc	0.603	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.07	J/mol×K	519.50	Joback Method
cpg	444.88	J/mol×K	656.37	Joback Method
cpg	433.16	J/mol×K	629.00	Joback Method
cpg	420.93	J/mol×K	601.62	Joback Method
cpg	408.18	J/mol×K	574.25	Joback Method
cpg	394.90	J/mol×K	546.87	Joback Method
cpg	456.11	J/mol×K	683.75	Joback Method
dvisc	0.0001109	Paxs	519.50	Joback Method

dvisc	0.0002007	Paxs	471.80	Joback Method
dvisc	0.0004150	Paxs	424.09	Joback Method
dvisc	0.0010317	Paxs	376.39	Joback Method
dvisc	0.0033408	Paxs	328.69	Joback Method
dvisc	0.0161218	Paxs	280.98	Joback Method
dvisc	0.1480969	Paxs	233.28	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.49962e+01
Coeff. B	-4.29835e+03
Coeff. C	-7.23660e+01
Temperature range (K), min.	364.60
Temperature range (K), max.	516.19

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19781272&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/45-189-3/3-Octanol-6-ethyl.pdf>

Generated by Cheméo on 2024-04-20 16:07:41.19586528 +0000 UTC m=+15918510.116442592.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.