3-Ethyl-4-octanol

Inchi: InChI=1S/C10H22O/c1-4-7-8-10(11)9(5-2)6-3/h9-11H,4-8H2,1-3H3
InchiKey: WXJDPIWUPZLVSF-UHFFFAOYSA-N
Formula: C10H22O
SMILES: CCCCC(O)C(CC)CC
Mol. weight [g/mol]: 158.28
CAS: 63126-48-7

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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.07	J/mol×K	519.50	Joback Method
cpg	394.90	J/mol×K	546.87	Joback Method
cpg	408.18	J/mol×K	574.25	Joback Method
cpg	420.93	J/mol×K	601.62	Joback Method
cpg	433.16	J/mol×K	629.00	Joback Method
cpg	444.88	J/mol×K	656.37	Joback Method
cpg	456.11	J/mol×K	683.75	Joback Method
dvisc	0.1480969	Pa×s	233.28	Joback Method
dvisc	0.0161218	Pa×s	280.98	Joback Method

dvisc	0.0033408	Pa×s	328.69	Joback Method
dvisc	0.0010317	Pa×s	376.39	Joback Method
dvisc	0.0004150	Pa×s	424.09	Joback Method
dvisc	0.0002007	Pa×s	471.80	Joback Method
dvisc	0.0001109	Pa×s	519.50	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44962e+01
Coeff. B	-4.10773e+03
Coeff. C	-7.06980e+01
Temperature range (K), min.	359.80
Temperature range (K), max.	517.93

Sources

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=C63126487&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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