2-Nonanol, 5-ethyl-

Other names: (3-Ethyl-n-heptyl)methylcarbinol
5-Ethyl-2-nonanol
5-ethylnonan-2-ol
Inchi: InChI=1S/C11H24O/c1-4-6-7-11(5-2)9-8-10(3)12/h10-12H,4-9H2,1-3H3
InchiKey: WYXKGYXADPUOOM-UHFFFAOYSA-N
Formula: C11H24O
SMILES: CCCCC(CC)CCC(C)O
Mol. weight [g/mol]: 172.31
CAS: 103-08-2

Physical Properties

Property code	Value	Unit	Source
gf	-99.96	kJ/mol	Joback Method
hf	-433.16	kJ/mol	Joback Method
hfus	21.29	kJ/mol	Joback Method
hvap	55.98	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.364		Crippen Method
mcvol	171.720	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
tb	498.00 ± 4.00	K	NIST Webbook
tc	705.81	K	Joback Method
tf	244.55	K	Joback Method
vc	0.658	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.18	J/mol×K	542.38	Joback Method
cpg	443.73	J/mol×K	569.62	Joback Method
cpg	457.69	J/mol×K	596.86	Joback Method
cpg	471.09	J/mol×K	624.10	Joback Method
cpg	483.93	J/mol×K	651.33	Joback Method
cpg	496.25	J/mol×K	678.57	Joback Method

cpg	508.04	J/mol×K	705.81	Joback Method
dvisc	0.1063589	Pa×s	244.55	Joback Method
dvisc	0.0121747	Pa×s	294.19	Joback Method
dvisc	0.0026058	Pa×s	343.83	Joback Method
dvisc	0.0008229	Pa×s	393.47	Joback Method
dvisc	0.0003364	Pa×s	443.10	Joback Method
dvisc	0.0001647	Pa×s	492.74	Joback Method
dvisc	0.0000919	Pa×s	542.38	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.63800e+01
Coeff. B	-4.92115e+03
Coeff. C	-7.95940e+01
Temperature range (K), min.	385.40
Temperature range (K), max.	524.20

Sources

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
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=C103082&Units=SI

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