5-Methyl-4-octanol

Inchi: InChI=1S/C9H20O/c1-4-6-8(3)9(10)7-5-2/h8-10H,4-7H2,1-3H3
InchiKey: YLTHHPQUTLMNIF-UHFFFAOYSA-N
Formula: C9H20O
SMILES: CCCC(C)C(O)CCC
Mol. weight [g/mol]: 144.25
CAS: 59734-23-5

Physical Properties

Property code	Value	Unit	Source
gf	-116.80	kJ/mol	Joback Method
hf	-391.88	kJ/mol	Joback Method
hfus	16.11	kJ/mol	Joback Method
hvap	51.53	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.584		Crippen Method
mcvol	143.540	ml/mol	McGowan Method
pc	2566.29	kPa	Joback Method
tb	496.62	K	Joback Method
tc	661.81	K	Joback Method
tf	222.01	K	Joback Method
vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.77	J/mol×K	496.62	Joback Method
cpg	347.81	J/mol×K	524.15	Joback Method
cpg	360.33	J/mol×K	551.68	Joback Method
cpg	372.35	J/mol×K	579.21	Joback Method
cpg	383.89	J/mol×K	606.75	Joback Method
cpg	394.96	J/mol×K	634.28	Joback Method
cpg	405.56	J/mol×K	661.81	Joback Method
dvisc	0.2091511	Pa×s	222.01	Joback Method
dvisc	0.0215322	Pa×s	267.78	Joback Method

dvisc	0.0043049	Pa×s	313.55	Joback Method
dvisc	0.0012970	Pa×s	359.31	Joback Method
dvisc	0.0005125	Pa×s	405.08	Joback Method
dvisc	0.0002445	Pa×s	450.85	Joback Method
dvisc	0.0001337	Pa×s	496.62	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52842e+01
Coeff. B	-4.24943e+03
Coeff. C	-6.76400e+01
Temperature range (K), min.	351.00
Temperature range (K), max.	493.75

Sources

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=C59734235&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