

2-Methyl-4-octanol

Inchi:	InChI=1S/C9H20O/c1-4-5-6-9(10)7-8(2)3/h8-10H,4-7H2,1-3H3
InchiKey:	BIAVIOIDPRPYJK-UHFFFAOYSA-N
Formula:	C9H20O
SMILES:	CCCCC(O)CC(C)C
Mol. weight [g/mol]:	144.26
CAS:	40575-41-5

Physical Properties

Property code	Value	Unit	Source
af	0.6249		Cheméo Relay (1.0)
gf	-116.80	kJ/mol	Joback Method
hf	-410.19	kJ/mol	Cheméo Relay (1.0)
hfus	16.11	kJ/mol	Joback Method
hvap	66.50	kJ/mol	Cheméo Relay (1.0)
ie	9.68	eV	Cheméo Relay (1.0)
log10ws	-2.46		Cheméo Relay (1.0)
logp	2.584		Crippen Method
mcvol	143.540	ml/mol	McGowan Method
pc	2566.29	kPa	Joback Method
tb	452.24	K	Cheméo Relay (1.0)
tc	628.24	K	Cheméo Relay (1.0)
tf	250.93	K	Cheméo Relay (1.0)
vc	0.538	m3/kmol	Cheméo Relay (1.0)

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	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.54889e+01
Coeff. B	-4.32451e+03
Coeff. C	-6.82380e+01
Temperature range (K), min.	352.72
Temperature range (K), max.	493.15

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40575415&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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

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