3-Octanol, 2,3-dimethyl-

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

Physical Properties

Property code	Value	Unit	Source
gf	-103.10	kJ/mol	Joback Method
hf	-415.99	kJ/mol	Joback Method
hfus	14.81	kJ/mol	Joback Method
hvap	52.85	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	2.974		Crippen Method
mcvol	157.630	ml/mol	McGowan Method
pc	2358.78	kPa	Joback Method
tb	462.25 ± 1.00	K	NIST Webbook
tc	686.53	K	Joback Method
tf	250.70	K	Joback Method
vc	0.598	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.78	J/mol×K	516.71	Joback Method
cpg	398.19	J/mol×K	545.01	Joback Method
cpg	411.92	J/mol×K	573.32	Joback Method
cpg	425.02	J/mol×K	601.62	Joback Method
cpg	437.50	J/mol×K	629.92	Joback Method
cpg	449.39	J/mol×K	658.22	Joback Method
cpg	460.72	J/mol×K	686.53	Joback Method
dvisc	0.0899105	Pa×s	250.70	Joback Method

dvisc	0.0128169	Pa×s	295.03	Joback Method
dvisc	0.0030395	Pa×s	339.37	Joback Method
dvisc	0.0010052	Pa×s	383.71	Joback Method
dvisc	0.0004181	Pa×s	428.04	Joback Method
dvisc	0.0002050	Pa×s	472.38	Joback Method
dvisc	0.0001136	Pa×s	516.71	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.64111e+01
Coeff. B	-4.62977e+03
Coeff. C	-6.96550e+01
Temperature range (K), min.	356.80
Temperature range (K), max.	486.77

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=C19781103&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

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