heptanol

Other names: heptan-1-ol
Inchi: InChI=1S/C7H16O/c1-2-3-4-5-6-7-8/h8H,2-7H2,1H3
InchiKey: BBMCTIGTTCKYKF-UHFFFAOYSA-N
Formula: C7H16O
SMILES: CCCCCCCO
Mol. weight [g/mol]: 116.20
CAS: 53535-33-4

Physical Properties

Property code	Value	Unit	Source
gf	-128.76	kJ/mol	Joback Method
hf	-340.04	kJ/mol	Joback Method
hfus	17.97	kJ/mol	Joback Method
hvap	47.86	kJ/mol	Joback Method
log10ws	-2.02		Crippen Method
logp	1.949		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	3093.29	kPa	Joback Method
rinpol	957.70		NIST Webbook
rinpol	959.50		NIST Webbook
rinpol	959.00		NIST Webbook
rinpol	958.20		NIST Webbook
rinpol	957.70		NIST Webbook
rinpol	942.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	951.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	974.00		NIST Webbook
rinpol	970.00		NIST Webbook
rinpol	970.00		NIST Webbook
rinpol	949.00		NIST Webbook
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ripol	1458.00		NIST Webbook
ripol	1443.00		NIST Webbook
ripol	1456.00		NIST Webbook
ripol	1463.00		NIST Webbook
ripol	1447.00		NIST Webbook
ripol	1425.00		NIST Webbook
tb	451.74	K	Joback Method
tc	612.20	K	Joback Method
tf	229.47	K	Joback Method
vc	0.447	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.80	J/mol×K	451.74	Joback Method
cpg	296.94	J/mol×K	585.45	Joback Method
cpg	287.84	J/mol×K	558.71	Joback Method
cpg	278.39	J/mol×K	531.97	Joback Method
cpg	268.58	J/mol×K	505.23	Joback Method
cpg	258.38	J/mol×K	478.48	Joback Method
cpg	305.68	J/mol×K	612.20	Joback Method
dvisc	0.0002110	Pa×s	451.74	Joback Method
dvisc	0.0003591	Pa×s	414.70	Joback Method
dvisc	0.0006783	Pa×s	377.65	Joback Method
dvisc	0.0014716	Pa×s	340.61	Joback Method
dvisc	0.0038567	Pa×s	303.56	Joback Method
dvisc	0.0132124	Pa×s	266.51	Joback Method
dvisc	0.0673608	Pa×s	229.47	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.09949e+01
Coeff. B	-5.80438e+03
Coeff. C	-6.60140e+01
Temperature range (K), min.	346.32
Temperature range (K), max.	436.11

Sources

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=C53535334&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

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume