5-Methyl-2-heptanol

Inchi: InChI=1S/C8H18O/c1-4-7(2)5-6-8(3)9/h7-9H,4-6H2,1-3H3
InchiKey: FYMBAYNKBWGEIK-UHFFFAOYSA-N
Formula: C8H18O
SMILES: CCC(C)CCC(C)O
Mol. weight [g/mol]: 130.23
CAS: 54630-50-1

Physical Properties

Property code	Value	Unit	Source
af	0.5993		Cheméo Relay (1.0)
gf	-125.22	kJ/mol	Joback Method
hf	-412.02	kJ/mol	Cheméo Relay (1.0)
hfus	13.52	kJ/mol	Joback Method
hvap	65.50	kJ/mol	Cheméo Relay (1.0)
ie	9.80	eV	Cheméo Relay (1.0)
log10ws	-1.91		Cheméo Relay (1.0)
logp	2.194		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
rinpol	856.00		NIST Webbook
ripol	1394.00		NIST Webbook
ripol	1395.00		NIST Webbook
ripol	1394.00		NIST Webbook
tb	445.05 ± 0.50	K	NIST Webbook
tc	615.97	K	Cheméo Relay (1.0)
tf	224.70	K	Cheméo Relay (1.0)
vc	0.473	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.45	J/mol×K	639.93	Joback Method
cpg	290.39	J/mol×K	473.74	Joback Method
cpg	302.54	J/mol×K	501.44	Joback Method

cpg	314.22	J/mol×K	529.14	Joback Method
cpg	325.44	J/mol×K	556.84	Joback Method
cpg	336.21	J/mol×K	584.53	Joback Method
cpg	346.54	J/mol×K	612.23	Joback Method
cpl	296.20	J/mol×K	298.50	NIST Webbook
dvisc	0.3001577	Pa×s	210.74	Joback Method
dvisc	0.0290327	Pa×s	254.57	Joback Method
dvisc	0.0055777	Pa×s	298.41	Joback Method
dvisc	0.0016351	Pa×s	342.24	Joback Method
dvisc	0.0006333	Pa×s	386.07	Joback Method
dvisc	0.0002977	Pa×s	429.91	Joback Method
dvisc	0.0001609	Pa×s	473.74	Joback Method
hvapt	51.90	kJ/mol	396.50	NIST Webbook
hvapt	47.20	kJ/mol	396.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.67459e+01
Coeff. B	-4.99895e+03
Coeff. C	-3.28520e+01
Temperature range (K), min.	336.59
Temperature range (K), max.	470.04

Sources

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=C54630501&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hvapt:	Enthalpy of vaporization at a given temperature
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
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