

4-Ethyl-4-heptanol

Other names:	4-Heptanol, 4-ethyl-
Inchi:	InChI=1S/C9H20O/c1-4-7-9(10,6-3)8-5-2/h10H,4-8H2,1-3H3
InchiKey:	GNROHGFUVTWFG-UHFFFAOYSA-N
Formula:	C9H20O
SMILES:	CCCC(O)(CC)CCC
Mol. weight [g/mol]:	144.25
CAS:	597-90-0

Physical Properties

Property code	Value	Unit	Source
gf	-109.08	kJ/mol	Joback Method
hf	-390.07	kJ/mol	Joback Method
hfus	15.74	kJ/mol	Joback Method
hvap	51.01	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.728		Crippen Method
mcvol	143.540	ml/mol	McGowan Method
pc	2574.11	kPa	Joback Method
tb	452.65 ± 5.00	K	NIST Webbook
tc	662.00	K	Joback Method
tf	254.43	K	Joback Method
vc	0.547	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.27	J/mol×K	494.27	Joback Method
cpg	350.61	J/mol×K	522.22	Joback Method
cpg	363.35	J/mol×K	550.18	Joback Method
cpg	375.49	J/mol×K	578.13	Joback Method
cpg	387.08	J/mol×K	606.09	Joback Method
cpg	398.12	J/mol×K	634.04	Joback Method
cpg	408.65	J/mol×K	662.00	Joback Method
dvisc	0.0562745	Paxs	254.43	Joback Method

dvisc	0.0106579	Paxs	294.40	Joback Method
dvisc	0.0030048	Paxs	334.38	Joback Method
dvisc	0.0011101	Paxs	374.35	Joback Method
dvisc	0.0004970	Paxs	414.32	Joback Method
dvisc	0.0002563	Paxs	454.30	Joback Method
dvisc	0.0001471	Paxs	494.27	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.63639e+01
Coeff. B	-4.53146e+03
Coeff. C	-6.68480e+01
Temperature range (K), min.	348.72
Temperature range (K), max.	476.85

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C597900&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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