

octyl

Inchi:	InChI=1S/C8H17/c1-3-5-7-8-6-4-2/h1,3-8H2,2H3
InchiKey:	AUNGTSCVKGQIAH-UHFFFAOYSA-N
Formula:	C8H17
SMILES:	[CH2]CCCCCCC
Mol. weight [g/mol]:	113.22
CAS:	4606-96-6

Physical Properties

Property code	Value	Unit	Source
gf	68.86	kJ/mol	Joback Method
hf	-152.64	kJ/mol	Joback Method
hfus	18.16	kJ/mol	Joback Method
hvap	33.26	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	3.181		Crippen Method
mcvol	121.430	ml/mol	McGowan Method
pc	2651.56	kPa	Joback Method
tb	381.74	K	Joback Method
tc	542.37	K	Joback Method
tf	196.29	K	Joback Method
vc	0.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.68	J/mol×K	381.74	Joback Method
cpg	284.08	J/mol×K	515.59	Joback Method
cpg	273.61	J/mol×K	488.82	Joback Method
cpg	262.66	J/mol×K	462.05	Joback Method
cpg	251.20	J/mol×K	435.28	Joback Method
cpg	239.22	J/mol×K	408.51	Joback Method
cpg	294.10	J/mol×K	542.37	Joback Method
dvisc	0.0003396	Pa×s	381.74	Joback Method
dvisc	0.0003909	Pa×s	350.83	Joback Method

dvisc	0.0004623	Pa×s	319.92	Joback Method
dvisc	0.0005668	Pa×s	289.01	Joback Method
dvisc	0.0007297	Pa×s	258.11	Joback Method
dvisc	0.0010062	Pa×s	227.20	Joback Method
dvisc	0.0015352	Pa×s	196.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4606966&Units=SI
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

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

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