

C6H11CH2OCH3

Inchi:	InChI=1S/C8H16O/c1-9-7-8-5-3-2-4-6-8/h8H,2-7H2,1H3
InchiKey:	UXXIFJBQPUDTNK-UHFFFAOYSA-N
Formula:	C8H16O
SMILES:	COCC1CCCCC1
Mol. weight [g/mol]:	128.21
CAS:	19752-94-4

Physical Properties

Property code	Value	Unit	Source
affp	833.50	kJ/mol	NIST Webbook
basg	801.60	kJ/mol	NIST Webbook
gf	-64.07	kJ/mol	Joback Method
hf	-286.35	kJ/mol	Joback Method
hfus	9.50	kJ/mol	Joback Method
hvap	36.24	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	2.213		Crippen Method
mcvol	118.590	ml/mol	McGowan Method
pc	3093.29	kPa	Joback Method
tb	424.41	K	Joback Method
tc	624.56	K	Joback Method
tf	209.53	K	Joback Method
vc	0.434	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.95	J/mol×K	424.41	Joback Method
cpg	255.92	J/mol×K	457.77	Joback Method
cpg	272.17	J/mol×K	491.13	Joback Method
cpg	287.70	J/mol×K	524.48	Joback Method
cpg	302.51	J/mol×K	557.84	Joback Method
cpg	316.61	J/mol×K	591.20	Joback Method
cpg	330.03	J/mol×K	624.56	Joback Method

dvisc	0.0058646	Paxs	209.53	Joback Method
dvisc	0.0023543	Paxs	245.34	Joback Method
dvisc	0.0011925	Paxs	281.16	Joback Method
dvisc	0.0007044	Paxs	316.97	Joback Method
dvisc	0.0004630	Paxs	352.78	Joback Method
dvisc	0.0003288	Paxs	388.60	Joback Method
dvisc	0.0002474	Paxs	424.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19752944&Units=SI
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

Legend

affp:	Proton affinity
basg:	Gas basicity
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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