CYCLOHEPTANEMETHANOL

Inchi: InChI=1S/C8H16O/c9-7-8-5-3-1-2-4-6-8/h8-9H,1-7H2
InchiKey: BMCQFFXPECPDPS-UHFFFAOYSA-N
Formula: C8H16O
SMILES: OCC1CCCCCC1
Mol. weight [g/mol]: 128.21

Physical Properties

Property code	Value	Unit	Source
af	0.5345		Cheméo Relay (1.0)
gf	-107.99	kJ/mol	Joback Method
hf	-304.89	kJ/mol	Cheméo Relay (1.0)
hfus	10.30	kJ/mol	Joback Method
hvap	67.87	kJ/mol	Cheméo Relay (1.0)
ie	9.61	eV	Cheméo Relay (1.0)
log10ws	-1.82		Cheméo Relay (1.0)
logp	1.949		Crippen Method
mcvol	118.590	ml/mol	McGowan Method
pc	3611.55	kPa	Joback Method
tb	478.91	K	Cheméo Relay (1.0)
tc	713.85	K	Cheméo Relay (1.0)
tf	300.04	K	Cheméo Relay (1.0)
vc	0.397	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.65	J/mol×K	498.44	Joback Method
cpg	290.40	J/mol×K	531.37	Joback Method
cpg	305.37	J/mol×K	564.30	Joback Method
cpg	319.57	J/mol×K	597.23	Joback Method
cpg	333.03	J/mol×K	630.16	Joback Method
cpg	345.75	J/mol×K	663.09	Joback Method
cpg	357.76	J/mol×K	696.02	Joback Method
dvisc	0.0923760	Pa×s	244.60	Joback Method

dvisc	0.0140749	Pa×s	286.91	Joback Method
dvisc	0.0034781	Pa×s	329.21	Joback Method
dvisc	0.0011817	Pa×s	371.52	Joback Method
dvisc	0.0005006	Pa×s	413.83	Joback Method
dvisc	0.0002487	Pa×s	456.13	Joback Method
dvisc	0.0001392	Pa×s	498.44	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	486.20	K	95.20	NIST Webbook

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):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4448753&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
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
ie: Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume