

2,4-Nonanediol, 5-ethyl-3-methyl-

Inchi:	InChI=1S/C12H26O2/c1-5-7-8-11(6-2)12(14)9(3)10(4)13/h9-14H,5-8H2,1-4H3
InchiKey:	LJGRJTMDBCJEG-UHFFFAOYSA-N
Formula:	C12H26O2
SMILES:	CCCCC(CC)C(O)C(C)C(C)O
Mol. weight [g/mol]:	202.33
CAS:	6628-31-5

Physical Properties

Property code	Value	Unit	Source
gf	-233.24	kJ/mol	Joback Method
hf	-616.59	kJ/mol	Joback Method
hfus	20.92	kJ/mol	Joback Method
hvap	74.11	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	2.581		Crippen Method
mcvol	191.680	ml/mol	McGowan Method
pc	2155.30	kPa	Joback Method
tb	656.56	K	Joback Method
tc	822.63	K	Joback Method
tf	286.64	K	Joback Method
vc	0.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.36	J/molxK	656.56	Joback Method
cpg	608.93	J/molxK	794.95	Joback Method
cpg	597.55	J/molxK	767.28	Joback Method
cpg	585.63	J/molxK	739.60	Joback Method
cpg	573.13	J/molxK	711.92	Joback Method
cpg	560.05	J/molxK	684.24	Joback Method
cpg	619.77	J/molxK	822.63	Joback Method
dvisc	0.0000128	Paxs	656.56	Joback Method
dvisc	0.0000283	Paxs	594.91	Joback Method

dvisc	0.0000752	Paxs	533.25	Joback Method
dvisc	0.0002580	Paxs	471.60	Joback Method
dvisc	0.0012835	Paxs	409.95	Joback Method
dvisc	0.0112672	Paxs	348.29	Joback Method
dvisc	0.2518162	Paxs	286.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6628315&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

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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