Octane-1,2,3,4-d9

Inchi: InChI=1S/C8H18/c1-3-5-7-8-6-4-2/h3-8H2,1-2H3/i1D3,3D2,5D2,7D2
InchiKey: TVMXDCGIABBOFY-NPNXCVMYSA-N
Formula: C8H9D9
SMILES: CCCCCCCC
Mol. weight [g/mol]: 123.28

Physical Properties

Property code	Value	Unit	Source
gf	16.48	kJ/mol	Joback Method
hf	-208.45	kJ/mol	Joback Method
hfus	16.48	kJ/mol	Joback Method
hvap	33.40	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	3.367		Crippen Method
mcvol	123.580	ml/mol	McGowan Method
pc	2535.37	kPa	Joback Method
rinpol	793.54		NIST Webbook
rinpol	793.54		NIST Webbook
tb	382.44	K	Joback Method
tc	545.88	K	Joback Method
tf	179.92	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.27	J/mol×K	382.44	Joback Method
cpg	245.27	J/mol×K	409.68	Joback Method
cpg	257.82	J/mol×K	436.92	Joback Method
cpg	269.93	J/mol×K	464.16	Joback Method
cpg	281.59	J/mol×K	491.40	Joback Method
cpg	292.83	J/mol×K	518.64	Joback Method
cpg	303.65	J/mol×K	545.88	Joback Method
dvisc	0.0056079	Pa×s	179.92	Joback Method

dvisc	0.0022039	Pa×s	213.67	Joback Method
dvisc	0.0011175	Pa×s	247.43	Joback Method
dvisc	0.0006670	Pa×s	281.18	Joback Method
dvisc	0.0004447	Pa×s	314.93	Joback Method
dvisc	0.0003207	Pa×s	348.69	Joback Method
dvisc	0.0002450	Pa×s	382.44	Joback Method

Sources

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=R136640&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume