

Octane-1,2,3,4,5,6-d13

Inchi:	InChI=1S/C8H18/c1-3-5-7-8-6-4-2/h3-8H2,1-2H3/i1D3,3D2,5D2,6D2,7D2,8D2
InchiKey:	TVMXDCGIABBOFY-SMTKFEHLSA-N
Formula:	C8H5D13
SMILES:	CCCCCCCC
Mol. weight [g/mol]:	127.31

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	790.86		NIST Webbook
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tb	382.44	K	Joback Method
tc	545.88	K	Joback Method
tf	179.92	K	Joback Method
vc	0.483	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0022039	Paxs	213.67	Joback Method
dvisc	0.0011175	Paxs	247.43	Joback Method
dvisc	0.0006670	Paxs	281.18	Joback Method
dvisc	0.0004447	Paxs	314.93	Joback Method
dvisc	0.0003207	Paxs	348.69	Joback Method
dvisc	0.0002450	Paxs	382.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R136635&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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