

Heptane-1,2,3,-d7

Inchi:	InChI=1S/C7H16/c1-3-5-7-6-4-2/h3-7H2,1-2H3/i1D3,3D2,5D2
InchiKey:	IMNFDUFMRHMDMM-HJHJEWFGSA-N
Formula:	C7H9D7
SMILES:	CCCCCCC
Mol. weight [g/mol]:	107.25

Physical Properties

Property code	Value	Unit	Source
gf	8.06	kJ/mol	Joback Method
hf	-187.81	kJ/mol	Joback Method
hfus	13.89	kJ/mol	Joback Method
hvap	31.18	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.977		Crippen Method
mcvol	109.490	ml/mol	McGowan Method
pc	2799.47	kPa	Joback Method
rinpola	694.77		NIST Webbook
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tb	359.56	K	Joback Method
tc	523.11	K	Joback Method
tf	168.65	K	Joback Method
vc	0.427	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.21	J/molxK	359.56	Joback Method
cpg	206.00	J/molxK	386.82	Joback Method
cpg	217.38	J/molxK	414.08	Joback Method
cpg	228.37	J/molxK	441.34	Joback Method
cpg	238.97	J/molxK	468.59	Joback Method
cpg	249.19	J/molxK	495.85	Joback Method
cpg	259.03	J/molxK	523.11	Joback Method
dvisc	0.0050984	Paxs	168.65	Joback Method

dvisc	0.0020471	Paxs	200.47	Joback Method
dvisc	0.0010554	Paxs	232.29	Joback Method
dvisc	0.0006383	Paxs	264.11	Joback Method
dvisc	0.0004301	Paxs	295.92	Joback Method
dvisc	0.0003129	Paxs	327.74	Joback Method
dvisc	0.0002409	Paxs	359.56	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R136586&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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