

Hephane-d16

Inchi:	InChI=1S/C6H12/c1-2-4-6-5-3-1/h1-6H2/i1D2,2D2,3D2
InchiKey:	XDTMQSROBMDMFD-NMFSSPJFSA-N
Formula:	C6H6D6
SMILES:	C1CCCCC1
Mol. weight [g/mol]:	90.20

Physical Properties

Property code	Value	Unit	Source
gf	31.80	kJ/mol	Joback Method
hf	-92.51	kJ/mol	Joback Method
hfus	2.06	kJ/mol	Joback Method
hvap	29.69	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	2.341		Crippen Method
mcvol	84.540	ml/mol	McGowan Method
pc	4130.29	kPa	Joback Method
rinpola	688.00		NIST Webbook
rinpola	688.00		NIST Webbook
tb	360.90	K	Joback Method
tc	565.41	K	Joback Method
tf	169.00	K	Joback Method
vc	0.305	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	134.03	J/molxK	360.90	Joback Method
cpg	148.78	J/molxK	394.98	Joback Method
cpg	162.77	J/molxK	429.07	Joback Method
cpg	176.04	J/molxK	463.15	Joback Method
cpg	188.60	J/molxK	497.24	Joback Method
cpg	200.49	J/molxK	531.32	Joback Method
cpg	211.71	J/molxK	565.41	Joback Method
dvisc	0.0153533	Paxs	169.00	Joback Method

dvisc	0.0047435	Paxs	200.98	Joback Method
dvisc	0.0020233	Paxs	232.97	Joback Method
dvisc	0.0010601	Paxs	264.95	Joback Method
dvisc	0.0006385	Paxs	296.93	Joback Method
dvisc	0.0004244	Paxs	328.92	Joback Method
dvisc	0.0003032	Paxs	360.90	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R136551&Units=SI

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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