

3,4-diethylhexa-1,5-diene

Inchi:	InChI=1S/C10H18/c1-5-9(6-2)10(7-3)8-4/h5,7,9-10H,1,3,6,8H2,2,4H3
InchiKey:	SLBUEUWNNTZSNQ-UHFFFAOYSA-N
Formula:	C10H18
SMILES:	C=CC(CC)C(C=C)CC
Mol. weight [g/mol]:	138.25

Physical Properties

Property code	Value	Unit	Source
gf	204.12	kJ/mol	Joback Method
hf	-9.43	kJ/mol	Joback Method
hfus	12.05	kJ/mol	Joback Method
hvap	35.74	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	3.411		Crippen Method
mcvol	143.160	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
rinpol	893.00		NIST Webbook
rinpol	898.00		NIST Webbook
rinpol	895.00		NIST Webbook
rinpol	894.00		NIST Webbook
rinpol	893.00		NIST Webbook
rinpol	894.00		NIST Webbook
rinpol	898.00		NIST Webbook
rinpol	900.00		NIST Webbook
ripol	952.00		NIST Webbook
ripol	952.00		NIST Webbook
tb	420.68	K	Joback Method
tc	597.23	K	Joback Method
tf	168.94	K	Joback Method
vc	0.545	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	283.09	J/molxK	420.68	Joback Method
cpg	298.03	J/molxK	450.11	Joback Method
cpg	312.32	J/molxK	479.53	Joback Method
cpg	325.96	J/molxK	508.96	Joback Method
cpg	338.98	J/molxK	538.38	Joback Method
cpg	351.41	J/molxK	567.81	Joback Method
cpg	363.27	J/molxK	597.23	Joback Method
dvisc	0.0148550	Paxs	168.94	Joback Method
dvisc	0.0036267	Paxs	210.90	Joback Method
dvisc	0.0014137	Paxs	252.85	Joback Method
dvisc	0.0007206	Paxs	294.81	Joback Method
dvisc	0.0004344	Paxs	336.77	Joback Method
dvisc	0.0002930	Paxs	378.72	Joback Method
dvisc	0.0002138	Paxs	420.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R285440&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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