

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
af	0.3044		Cheméo Relay (1.0)
hfus	12.05	kJ/mol	Joback Method
hvap	46.17	kJ/mol	Cheméo Relay (1.0)
ie	9.01	eV	Cheméo Relay (1.0)
logp	3.411		Crippen Method
mcvol	143.160	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
rinpol	893.00		NIST Webbook
rinpol	895.00		NIST Webbook
rinpol	894.00		NIST Webbook
rinpol	893.00		NIST Webbook
rinpol	900.00		NIST Webbook
rinpol	898.00		NIST Webbook
rinpol	894.00		NIST Webbook
rinpol	898.00		NIST Webbook
ripol	952.00		NIST Webbook
ripol	952.00		NIST Webbook
tb	425.59	K	Cheméo Relay (1.0)
tc	579.86	K	Cheméo Relay (1.0)
tf	191.29	K	Cheméo Relay (1.0)
vc	0.493	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.09	J/mol×K	420.68	Joback Method

cpg	298.03	J/mol×K	450.11	Joback Method
cpg	312.32	J/mol×K	479.53	Joback Method
cpg	325.96	J/mol×K	508.96	Joback Method
cpg	338.98	J/mol×K	538.38	Joback Method
cpg	351.41	J/mol×K	567.81	Joback Method
cpg	363.27	J/mol×K	597.23	Joback Method
dvisc	0.0148550	Pa×s	168.94	Joback Method
dvisc	0.0036267	Pa×s	210.90	Joback Method
dvisc	0.0014137	Pa×s	252.85	Joback Method
dvisc	0.0007206	Pa×s	294.81	Joback Method
dvisc	0.0004344	Pa×s	336.77	Joback Method
dvisc	0.0002930	Pa×s	378.72	Joback Method
dvisc	0.0002138	Pa×s	420.68	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R285440&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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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