Hexane, 3,3-diethyl-

Other names: 3,3-Diethylhexane
Inchi: InChI=1S/C10H22/c1-5-9-10(6-2,7-3)8-4/h5-9H2,1-4H3
InchiKey: WWNGLKDLYKNGGT-UHFFFAOYSA-N
Formula: C10H22
SMILES: CCCC(CC)(CC)CC
Mol. weight [g/mol]: 142.28
CAS: 17302-02-2

Physical Properties

Property code	Value	Unit	Source
gf	36.16	kJ/mol	Joback Method
hf	-258.48	kJ/mol	Joback Method
hfus	14.24	kJ/mol	Joback Method
hvap	36.56	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	4.003		Crippen Method
mcvol	151.760	ml/mol	McGowan Method
pc	2145.33	kPa	Joback Method
rinpol	954.00		NIST Webbook
tb	424.97	K	Joback Method
tc	597.50	K	Joback Method
tf	204.88	K	Joback Method
vc	0.585	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.97	J/mol×K	424.97	Joback Method
cpg	333.53	J/mol×K	453.73	Joback Method
cpg	349.34	J/mol×K	482.48	Joback Method
cpg	364.44	J/mol×K	511.24	Joback Method
cpg	378.86	J/mol×K	539.99	Joback Method
cpg	392.61	J/mol×K	568.75	Joback Method
cpg	405.72	J/mol×K	597.50	Joback Method

dvisc	0.0108562	Pa×s	204.88	Joback Method
dvisc	0.0035911	Pa×s	241.56	Joback Method
dvisc	0.0015903	Pa×s	278.24	Joback Method
dvisc	0.0008514	Pa×s	314.92	Joback Method
dvisc	0.0005192	Pa×s	351.61	Joback Method
dvisc	0.0003477	Pa×s	388.29	Joback Method
dvisc	0.0002495	Pa×s	424.97	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol143.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17302022&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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