

3,4-Diethyl-2-hexene(E)

Inchi:	InChI=1S/C10H20/c1-5-9(6-2)10(7-3)8-4/h5,10H,6-8H2,1-4H3/b9-5+
InchiKey:	WTCHQGKPTSGKHU-WEVVVXLNSA-N
Formula:	C10H20
SMILES:	CC=C(CC)C(CC)CC
Mol. weight [g/mol]:	140.27
CAS:	59643-70-8

Physical Properties

Property code	Value	Unit	Source
gf	102.55	kJ/mol	Joback Method
hf	-147.58	kJ/mol	Joback Method
hfus	17.03	kJ/mol	Joback Method
hvap	37.50	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.779		Crippen Method
mcvol	147.460	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
tb	431.80	K	Joback Method
tc	609.06	K	Joback Method
tf	168.42	K	Joback Method
vc	0.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.23	J/molxK	431.80	Joback Method
cpg	315.85	J/molxK	461.34	Joback Method
cpg	330.80	J/molxK	490.89	Joback Method
cpg	345.08	J/molxK	520.43	Joback Method
cpg	358.72	J/molxK	549.97	Joback Method
cpg	371.75	J/molxK	579.52	Joback Method
cpg	384.19	J/molxK	609.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59643708&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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