

3-Ethyl-1,5-octadiene, isomer

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

Physical Properties

Property code	Value	Unit	Source
gf	198.94	kJ/mol	Joback Method
hf	-12.36	kJ/mol	Joback Method
hfus	17.06	kJ/mol	Joback Method
hvap	36.75	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.555		Crippen Method
mcvol	143.160	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
rinpol	949.00		NIST Webbook
rinpol	949.00		NIST Webbook
rinpol	949.00		NIST Webbook
tb	428.60	K	Joback Method
tc	606.13	K	Joback Method
tf	180.62	K	Joback Method
vc	0.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.09	J/mol×K	428.60	Joback Method
cpg	298.96	J/mol×K	458.19	Joback Method
cpg	313.14	J/mol×K	487.78	Joback Method
cpg	326.65	J/mol×K	517.36	Joback Method
cpg	339.54	J/mol×K	546.95	Joback Method
cpg	351.81	J/mol×K	576.54	Joback Method
cpg	363.50	J/mol×K	606.13	Joback Method

dvisc	0.0087656	Pa×s	180.62	Joback Method
dvisc	0.0025414	Pa×s	221.95	Joback Method
dvisc	0.0010869	Pa×s	263.28	Joback Method
dvisc	0.0005853	Pa×s	304.61	Joback Method
dvisc	0.0003655	Pa×s	345.94	Joback Method
dvisc	0.0002523	Pa×s	387.27	Joback Method
dvisc	0.0001871	Pa×s	428.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R288692&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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