2,4-Octadiene

Other names: 2,4-Octadiene mixture
Inchi: InChI=1S/C8H14/c1-3-5-7-8-6-4-2/h3,5,7-8H,4,6H2,1-2H3/b5-3+,8-7+
InchiKey: NZLCAHVLJPDRBL-VSAQMIDASA-N
Formula: C8H14
SMILES: CC=CC=CCCC
Mol. weight [g/mol]: 110.20
CAS: 13643-08-8

Physical Properties

Property code	Value	Unit	Source
gf	176.92	kJ/mol	Joback Method
hf	25.99	kJ/mol	Joback Method
hfus	16.88	kJ/mol	Joback Method
hvap	33.32	kJ/mol	Joback Method
ie	8.13	eV	NIST Webbook
log10ws	-2.88		Crippen Method
logp	2.919		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	2823.32	kPa	Joback Method
rinpol	811.00		NIST Webbook
rinpol	819.00		NIST Webbook
rinpol	815.00		NIST Webbook
rinpol	819.00		NIST Webbook
rinpol	818.00		NIST Webbook
rinpol	815.00		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	811.00		NIST Webbook
ripol	919.00		NIST Webbook
ripol	886.00		NIST Webbook
ripol	919.00		NIST Webbook
ripol	930.00		NIST Webbook
tb	406.00 ± 3.00	K	NIST Webbook
tb	405.20 ± 2.00	K	NIST Webbook
tb	406.90 ± 3.00	K	NIST Webbook
tc	571.58	K	Joback Method
tf	169.76	K	Joback Method
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.62	J/mol×K	390.76	Joback Method
cpg	216.35	J/mol×K	420.90	Joback Method
cpg	228.43	J/mol×K	451.03	Joback Method
cpg	239.90	J/mol×K	481.17	Joback Method
cpg	250.79	J/mol×K	511.30	Joback Method
cpg	261.13	J/mol×K	541.44	Joback Method
cpg	270.94	J/mol×K	571.58	Joback Method
dvisc	0.0049045	Pa×s	169.76	Joback Method
dvisc	0.0016869	Pa×s	206.59	Joback Method
dvisc	0.0008014	Pa×s	243.43	Joback Method
dvisc	0.0004630	Pa×s	280.26	Joback Method
dvisc	0.0003039	Pa×s	317.09	Joback Method
dvisc	0.0002177	Pa×s	353.93	Joback Method
dvisc	0.0001661	Pa×s	390.76	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13643088&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

ie:	Ionization energy
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