1,3-Octadiene

Inchi: InChI=1S/C8H14/c1-3-5-7-8-6-4-2/h3,5,7H,1,4,6,8H2,2H3
InchiKey: QTYUSOHYEPOHLV-UHFFFAOYSA-N
Formula: C8H14
SMILES: C=CC=CCCCC
Mol. weight [g/mol]: 110.20
CAS: 1002-33-1

Physical Properties

Property code	Value	Unit	Source
gf	184.54	kJ/mol	Joback Method
hf	34.20	kJ/mol	Joback Method
hfus	15.40	kJ/mol	Joback Method
hvap	32.69	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.919		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	2793.56	kPa	Joback Method
rinpol	819.00		NIST Webbook
rinpol	829.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	825.00		NIST Webbook
rinpol	827.00		NIST Webbook
rinpol	827.00		NIST Webbook
rinpol	825.00		NIST Webbook
rinpol	830.00		NIST Webbook
rinpol	819.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	777.10		NIST Webbook
rinpol	829.00		NIST Webbook
rinpol	827.00		NIST Webbook
rinpol	826.00		NIST Webbook
rinpol	827.00		NIST Webbook
rinpol	827.00		NIST Webbook
rinpol	777.10		NIST Webbook
ripol	958.00		NIST Webbook
ripol	954.00		NIST Webbook

ripol	954.00		NIST Webbook
tb	383.28	K	Joback Method
tc	558.73	K	Joback Method
tf	173.08	K	Joback Method
vc	0.445	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.47	J/mol×K	383.28	Joback Method
cpg	259.71	J/mol×K	529.49	Joback Method
cpg	249.52	J/mol×K	500.25	Joback Method
cpg	238.82	J/mol×K	471.01	Joback Method
cpg	227.59	J/mol×K	441.76	Joback Method
cpg	215.81	J/mol×K	412.52	Joback Method
cpg	269.43	J/mol×K	558.73	Joback Method
dvisc	0.0001960	Pa×s	383.28	Joback Method
dvisc	0.0002531	Pa×s	348.25	Joback Method
dvisc	0.0003462	Pa×s	313.21	Joback Method
dvisc	0.0005124	Pa×s	278.18	Joback Method
dvisc	0.0008489	Pa×s	243.15	Joback Method
dvisc	0.0016670	Pa×s	208.11	Joback Method
dvisc	0.0043022	Pa×s	173.08	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1002331&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume