1,7-Octadiene

Other names:	.alpha.,.omega.-octadiene
	Octa-1,7-diene
	octadiene-1,7
	«alpha»,«omega»-Octadiene
	Â«alphaÂ»,Â«omegaÂ»-Octadiene
Inchi:	InChI=1S/C8H14/c1-3-5-7-8-6-4-2/h3-4H,1-2,5-8H2
InchiKey:	XWJBRBSPAODJER-UHFFFAOYSA-N
Formula:	C8H14
SMILES:	C=CCCCCC=C
Mol. weight [g/mol]:	110.20
CAS:	3710-30-3

Physical Properties

Property code	Value	Unit	Source
gf	192.16	kJ/mol	Joback Method
hf	42.41	kJ/mol	Joback Method
hfus	13.92	kJ/mol	Joback Method
hvap	32.06	kJ/mol	Joback Method
ie	9.52 ± 0.02	eV	NIST Webbook
log10ws	-2.88		Crippen Method
logp	2.919		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
rinpol	767.80		NIST Webbook
rinpol	764.20		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	762.00		NIST Webbook
rinpol	764.99		NIST Webbook
rinpol	764.99		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	778.00		NIST Webbook
rinpol	795.00		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	763.50		NIST Webbook
rinpol	762.60		NIST Webbook
rinpol	763.50		NIST Webbook
rinpol	762.60		NIST Webbook

rinpol	782.00		NIST Webbook
tb	390.70	K	NIST Webbook
tb	387.00	K	NIST Webbook
tb	388.70	K	NIST Webbook
tb	388.00 ± 4.00	K	NIST Webbook
tb	390.00 ± 3.00	K	NIST Webbook
tb	389.00 ± 2.00	K	NIST Webbook
tc	546.00	K	Joback Method
tf	176.40	K	Joback Method
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.37	J/mol×K	375.80	Joback Method
cpg	215.33	J/mol×K	404.17	Joback Method
cpg	226.78	J/mol×K	432.53	Joback Method
cpg	237.74	J/mol×K	460.90	Joback Method
cpg	248.23	J/mol×K	489.26	Joback Method
cpg	258.27	J/mol×K	517.63	Joback Method
cpg	267.87	J/mol×K	546.00	Joback Method
dvisc	0.0038245	Pa×s	176.40	Joback Method
dvisc	0.0016530	Pa×s	209.63	Joback Method
dvisc	0.0008988	Pa×s	242.87	Joback Method
dvisc	0.0005659	Pa×s	276.10	Joback Method
dvisc	0.0003936	Pa×s	309.33	Joback Method
dvisc	0.0002937	Pa×s	342.57	Joback Method
dvisc	0.0002308	Pa×s	375.80	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55248e+01
Coeff. B	-3.70607e+03
Coeff. C	-4.91950e+01
Temperature range (K), min.	292.42

Temperature range (K), max.	412.06

Sources

Thermodynamics of solvation in propylene glycol and methyl cellosolve:	https://www.doi.org/10.1016/j.jct.2014.06.006
Abraham model correlations for describing the thermodynamic properties of solute transfer into pentyl acetate based on headspace chromatographic and solubility measurements:	https://www.doi.org/10.1016/j.jct.2018.05.003
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3710303&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume