trans-3,trans-5-octadiene

Other names: 3,5-Octadiene, (E,E)
Inchi: InChI=1S/C8H14/c1-3-5-7-8-6-4-2/h5-8H,3-4H2,1-2H3/b7-5+,8-6+
InchiKey: HWXQYUCHSICMAS-KQQUZDAGSA-N
Formula: C8H14
SMILES: CC/C=C/C=C/CC
Mol. weight [g/mol]: 110.20

Physical Properties

Property code	Value	Unit	Source
af	0.2453		Cheméo Relay (1.0)
gf	176.92	kJ/mol	Joback Method
hf	-6.96	kJ/mol	Cheméo Relay (1.0)
hfus	16.88	kJ/mol	Joback Method
hvap	41.32	kJ/mol	Cheméo Relay (1.0)
ie	8.02	eV	Cheméo Relay (1.0)
logp	2.919		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	2823.32	kPa	Joback Method
rinpol	838.10		NIST Webbook
rinpol	843.30		NIST Webbook
rinpol	838.70		NIST Webbook
rinpol	837.00		NIST Webbook
rinpol	838.10		NIST Webbook
tb	389.90	K	Cheméo Relay (1.0)
tc	577.60	K	Cheméo Relay (1.0)
tf	226.07	K	Cheméo Relay (1.0)
vc	0.433	m3/kmol	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K

Coeff. A	-3.27480e+01
Coeff. B	8.03840e-01
Coeff. C	-5.79000e-04
Coeff. D	1.78800e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Information	Value
Property code	dvisc
Equation	Y = exp(A + B/T + C·ln(T) + D·T^E)
Y unit	Pa×s
Coeff. A	-1.13037e+01
Coeff. B	1.01620e+03
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Basis	predicted
Comment	Liquid phase. Joback/Reid (1987), valid from Tf to 0.7·Tc.
Temperature range (K), min.	169.76
Temperature range (K), max.	400.31

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R138220&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af: Acentric Factor
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
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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