1,3-trans,5-cis-Octatriene

Other names: 1,3,5-Octatriene, (E,Z)-
(3E,5Z)-1,3,5-Octatriene
1,3-(E)-5-(Z)-Octatriene
(E,Z)-1,3,5-Octatriene
Sarohornene C
1,(E)-3,(Z)-5-Octatriene
Inchi: InChI=1S/C8H12/c1-3-5-7-8-6-4-2/h3,5-8H,1,4H2,2H3/b7-5+,8-6-
InchiKey: HOXGZVUCAYFWGR-YMBWGVAGSA-N
Formula: C8H12
SMILES: C=CC=CC=CCC
Mol. weight [g/mol]: 108.18
CAS: 40087-61-4

Physical Properties

Property code	Value	Unit	Source
gf	264.76	kJ/mol	Joback Method
hf	151.42	kJ/mol	Joback Method
hfus	15.60	kJ/mol	Joback Method
hvap	32.65	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.695		Crippen Method
mcvol	110.680	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
rinpol	920.00		NIST Webbook
rinpol	880.00		NIST Webbook
ripol	1109.00		NIST Webbook
ripol	1108.00		NIST Webbook
ripol	1097.00		NIST Webbook
ripol	1114.00		NIST Webbook
ripol	1108.00		NIST Webbook
tb	387.44	K	Joback Method
tc	572.16	K	Joback Method
tf	168.00	K	Joback Method
vc	0.424	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.00	J/mol×K	387.44	Joback Method
cpg	201.15	J/mol×K	418.23	Joback Method
cpg	212.62	J/mol×K	449.01	Joback Method
cpg	223.45	J/mol×K	479.80	Joback Method
cpg	233.67	J/mol×K	510.59	Joback Method
cpg	243.32	J/mol×K	541.37	Joback Method
cpg	252.44	J/mol×K	572.16	Joback Method
dvisc	0.0039890	Pa×s	168.00	Joback Method
dvisc	0.0014499	Pa×s	204.57	Joback Method
dvisc	0.0007163	Pa×s	241.15	Joback Method
dvisc	0.0004262	Pa×s	277.72	Joback Method
dvisc	0.0002861	Pa×s	314.29	Joback Method
dvisc	0.0002087	Pa×s	350.87	Joback Method
dvisc	0.0001616	Pa×s	387.44	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C40087614&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