1,3,7-Octatriene

Other names: «alpha»-Ocimene
octa-1,3,7-triene
Inchi: InChI=1S/C8H12/c1-3-5-7-8-6-4-2/h3-5,7H,1-2,6,8H2
InchiKey: ZTJHDEXGCKAXRZ-UHFFFAOYSA-N
Formula: C8H12
SMILES: C=CC=CCCC=C
Mol. weight [g/mol]: 108.18
CAS: 1002-35-3

Physical Properties

Property code	Value	Unit	Source
gf	272.38	kJ/mol	Joback Method
hf	159.63	kJ/mol	Joback Method
hfus	14.12	kJ/mol	Joback Method
hvap	32.02	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.695		Crippen Method
mcvol	110.680	ml/mol	McGowan Method
pc	2921.84	kPa	Joback Method
rinpol	808.00		NIST Webbook
rinpol	805.00		NIST Webbook
rinpol	805.00		NIST Webbook
ripol	1249.00		NIST Webbook
tb	393.00 ± 4.00	K	NIST Webbook
tc	559.15	K	Joback Method
tf	171.32	K	Joback Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.08	J/mol×K	379.96	Joback Method
cpg	242.22	J/mol×K	529.28	Joback Method
cpg	232.69	J/mol×K	499.42	Joback Method

cpg	222.63	J/mol×K	469.55	Joback Method
cpg	212.03	J/mol×K	439.69	Joback Method
cpg	200.86	J/mol×K	409.82	Joback Method
cpg	251.26	J/mol×K	559.15	Joback Method
dvisc	0.0001901	Pa×s	379.96	Joback Method
dvisc	0.0002419	Pa×s	345.19	Joback Method
dvisc	0.0003250	Pa×s	310.41	Joback Method
dvisc	0.0004703	Pa×s	275.64	Joback Method
dvisc	0.0007574	Pa×s	240.87	Joback Method
dvisc	0.0014324	Pa×s	206.09	Joback Method
dvisc	0.0035085	Pa×s	171.32	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C1002353&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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