2,5-dimethyl-1,3,5-hexatriene

Inchi: InChI=1S/C8H12/c1-7(2)5-6-8(3)4/h5-6H,1,3H2,2,4H3
InchiKey: ZVFFWOKVVPSTAL-UHFFFAOYSA-N
Formula: C8H12
SMILES: C=C(C)C=CC(=C)C
Mol. weight [g/mol]: 108.18
CAS: 4916-63-6

Physical Properties

Property code	Value	Unit	Source
gf	255.28	kJ/mol	Joback Method
hf	140.05	kJ/mol	Joback Method
hfus	11.50	kJ/mol	Joback Method
hvap	32.18	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
tb	398.00 ± 4.00	K	NIST Webbook
tc	566.32	K	Joback Method
tf	143.40	K	Joback Method
vc	0.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.07	J/mol×K	379.72	Joback Method
cpg	201.26	J/mol×K	410.82	Joback Method
cpg	212.80	J/mol×K	441.92	Joback Method
cpg	223.72	J/mol×K	473.02	Joback Method
cpg	234.05	J/mol×K	504.12	Joback Method
cpg	243.82	J/mol×K	535.22	Joback Method
cpg	253.07	J/mol×K	566.32	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.76927e+01
Coeff. B	-4.44955e+03
Coeff. C	-5.76740e+01
Temperature range (K), min.	313.32
Temperature range (K), max.	417.05

Sources

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
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=C4916636&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume