1,4,6-Octatriene, 2,7-dimethyl

Inchi: InChI=1S/C10H16/c1-9(2)7-5-6-8-10(3)4/h5-6,8H,1,7H2,2-4H3/b6-5+
InchiKey: PHYKXFWYIKUYFR-AATRIKPKSA-N
Formula: C10H16
SMILES: C=C(C)CC=CC=C(C)C
Mol. weight [g/mol]: 136.23

Physical Properties

Property code	Value	Unit	Source
gf	264.50	kJ/mol	Joback Method
hf	90.56	kJ/mol	Joback Method
hfus	18.16	kJ/mol	Joback Method
hvap	37.26	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.475		Crippen Method
mcvol	138.860	ml/mol	McGowan Method
pc	2445.89	kPa	Joback Method
rinpol	988.00		NIST Webbook
tb	432.96	K	Joback Method
tc	622.27	K	Joback Method
tf	162.62	K	Joback Method
vc	0.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.68	J/mol×K	432.96	Joback Method
cpg	283.41	J/mol×K	464.51	Joback Method
cpg	297.33	J/mol×K	496.06	Joback Method
cpg	310.50	J/mol×K	527.62	Joback Method
cpg	322.94	J/mol×K	559.17	Joback Method
cpg	334.71	J/mol×K	590.72	Joback Method
cpg	345.84	J/mol×K	622.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R3575&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume