1,4-Pentadiene, 2,3,3-trimethyl-

Other names: 2,3,3-Trimethyl-1,4-pentadiene
Inchi: InChI=1S/C8H14/c1-6-8(4,5)7(2)3/h6H,1-2H2,3-5H3
InchiKey: OXYDHUPSYIQGAP-UHFFFAOYSA-N
Formula: C8H14
SMILES: C=CC(C)(C)C(=C)C
Mol. weight [g/mol]: 110.20
CAS: 756-02-5

Physical Properties

Property code	Value	Unit	Source
gf	186.45	kJ/mol	Joback Method
hf	23.87	kJ/mol	Joback Method
hfus	5.19	kJ/mol	Joback Method
hvap	30.85	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.775		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
rinpol	817.00		NIST Webbook
tb	372.45	K	Joback Method
tc	557.91	K	Joback Method
tf	164.86	K	Joback Method
vc	0.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.26	J/mol×K	372.45	Joback Method
cpg	218.07	J/mol×K	403.36	Joback Method
cpg	231.12	J/mol×K	434.27	Joback Method
cpg	243.44	J/mol×K	465.18	Joback Method
cpg	255.06	J/mol×K	496.09	Joback Method
cpg	266.03	J/mol×K	527.00	Joback Method
cpg	276.38	J/mol×K	557.91	Joback Method

Sources

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=C756025&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume