2,3,4-HEXATRIENE, 2,5-DIMETHYL-

Inchi: InChI=1S/C8H12/c1-7(2)5-6-8(3)4/h1-4H3
InchiKey: SOESISOWJSWAJZ-UHFFFAOYSA-N
Formula: C8H12
SMILES: CC(C)=C=C=C(C)C
Mol. weight [g/mol]: 108.18

Physical Properties

Property code	Value	Unit	Source
af	0.1608		Cheméo Relay (1.0)
gf	336.16	kJ/mol	Joback Method
hf	208.75	kJ/mol	Cheméo Relay (1.0)
hfus	18.32	kJ/mol	Joback Method
hvap	38.68	kJ/mol	Cheméo Relay (1.0)
ie	7.70	eV	NIST Webbook
logp	2.673		Crippen Method
mcvol	110.680	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
tb	391.08	K	Cheméo Relay (1.0)
tc	564.97	K	Cheméo Relay (1.0)
tf	294.88	K	Cheméo Relay (1.0)
vc	0.416	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.64	J/mol×K	392.90	Joback Method
cpg	210.92	J/mol×K	426.81	Joback Method
cpg	221.81	J/mol×K	460.73	Joback Method
cpg	232.29	J/mol×K	494.64	Joback Method
cpg	242.38	J/mol×K	528.56	Joback Method
cpg	252.07	J/mol×K	562.47	Joback Method
cpg	261.36	J/mol×K	596.39	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2431314&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
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
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume