1,6-Octadiene, 2,5-dimethyl-, (E)-

Other names: (6E)-2,5-Dimethyl-1,6-octadiene
(E)-2,5-Dimethyl-1,6-octadiene
Inchi: InChI=1S/C10H18/c1-5-6-10(4)8-7-9(2)3/h5-6,10H,2,7-8H2,1,3-4H3/b6-5+
InchiKey: FBNUSKGBPHDTRX-AATRIKPKSA-N
Formula: C10H18
SMILES: C=C(C)CCC(C)C=CC
Mol. weight [g/mol]: 138.25
CAS: 68702-25-0

Physical Properties

Property code	Value	Unit	Source
gf	190.39	kJ/mol	Joback Method
hf	-22.15	kJ/mol	Joback Method
hfus	15.74	kJ/mol	Joback Method
hvap	36.83	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.555		Crippen Method
mcvol	143.160	ml/mol	McGowan Method
pc	2331.52	kPa	Joback Method
rinpol	911.00		NIST Webbook
rinpol	911.00		NIST Webbook
tb	428.48	K	Joback Method
tc	609.41	K	Joback Method
tf	166.66	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.02	J/mol×K	428.48	Joback Method
cpg	299.14	J/mol×K	458.64	Joback Method
cpg	313.54	J/mol×K	488.79	Joback Method
cpg	327.26	J/mol×K	518.95	Joback Method
cpg	340.32	J/mol×K	549.10	Joback Method

cpg	352.75	J/mol×K	579.26	Joback Method
cpg	364.58	J/mol×K	609.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C68702250&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

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