2,6-Octadiene, 2,7-dimethyl-

Other names:	2,7-Dimethyl-2,6-octadiene
Inchi:	InChI=1S/C10H18/c1-9(2)7-5-6-8-10(3)4/h7-8H,5-6H2,1-4H3
InchiKey:	PSOPUECGKNQIPH-UHFFFAOYSA-N
Formula:	C10H18
SMILES:	CC(C)=CCCC=C(C)C
Mol. weight [g/mol]:	138.25
CAS:	16736-42-8

Physical Properties

Property code	Value	Unit	Source
gf	176.66	kJ/mol	Joback Method
hf	-34.87	kJ/mol	Joback Method
hfus	19.44	kJ/mol	Joback Method
hvap	37.93	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	3.699		Crippen Method
mcvol	143.160	ml/mol	McGowan Method
pc	2347.36	kPa	Joback Method
tb	436.28	K	Joback Method
tc	621.64	K	Joback Method
tf	164.38	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.91	J/mol×K	436.28	Joback Method
cpg	300.18	J/mol×K	467.17	Joback Method
cpg	314.68	J/mol×K	498.07	Joback Method
cpg	328.46	J/mol×K	528.96	Joback Method
cpg	341.53	J/mol×K	559.86	Joback Method
cpg	353.94	J/mol×K	590.75	Joback Method
cpg	365.73	J/mol×K	621.64	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54106e+01
Coeff. B	-4.07695e+03
Coeff. C	-6.32340e+01
Temperature range (K), min.	332.82
Temperature range (K), max.	466.93

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=C16736428&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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