

4-Octene, 2,6-dimethyl-, [S-(E)]-

Other names:	(S,E)-2,6-Dimethyloct-4-ene
Inchi:	InChI=1S/C10H20/c1-5-10(4)8-6-7-9(2)3/h6,8-10H,5,7H2,1-4H3/b8-6+/t10-/m1/s1
InchiKey:	PBPBSFCZFRLBFJ-QEHWCHDUSA-N
Formula:	C10H20
SMILES:	CCC(C)C=CCC(C)C
Mol. weight [g/mol]:	140.27
CAS:	62960-76-3

Physical Properties

Property code	Value	Unit	Source
gf	108.66	kJ/mol	Joback Method
hf	-143.07	kJ/mol	Joback Method
hfus	14.81	kJ/mol	Joback Method
hvap	37.04	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	3.635		Crippen Method
mcvol	147.460	ml/mol	McGowan Method
pc	2246.13	kPa	Joback Method
rinpol	911.10		NIST Webbook
tb	431.48	K	Joback Method
tc	609.35	K	Joback Method
tf	167.38	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.30	J/mol×K	431.48	Joback Method
cpg	316.10	J/mol×K	461.12	Joback Method
cpg	331.20	J/mol×K	490.77	Joback Method
cpg	345.63	J/mol×K	520.41	Joback Method
cpg	359.41	J/mol×K	550.06	Joback Method
cpg	372.56	J/mol×K	579.70	Joback Method
cpg	385.12	J/mol×K	609.35	Joback Method

dvisc	0.0212319	Pa×s	167.38	Joback Method
dvisc	0.0041931	Pa×s	211.40	Joback Method
dvisc	0.0014484	Pa×s	255.41	Joback Method
dvisc	0.0006839	Pa×s	299.43	Joback Method
dvisc	0.0003914	Pa×s	343.45	Joback Method
dvisc	0.0002543	Pa×s	387.46	Joback Method
dvisc	0.0001804	Pa×s	431.48	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=C62960763&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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