

2-Octene, 2,7-dimethyl-

Inchi:	InChI=1S/C10H20/c1-9(2)7-5-6-8-10(3)4/h7,10H,5-6,8H2,1-4H3
InchiKey:	NRQAGCXZYXDTPS-UHFFFAOYSA-N
Formula:	C10H20
SMILES:	CC(C)=CCCC(C)C
Mol. weight [g/mol]:	140.27
CAS:	2050-81-9

Physical Properties

Property code	Value	Unit	Source
gf	102.55	kJ/mol	Joback Method
hf	-147.58	kJ/mol	Joback Method
hfus	17.03	kJ/mol	Joback Method
hvap	37.50	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.779		Crippen Method
mcvol	147.460	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
tb	430.15 ± 2.00	K	NIST Webbook
tb	435.00 ± 6.00	K	NIST Webbook
tc	609.06	K	Joback Method
tf	193.70 ± 5.00	K	NIST Webbook
vc	0.571	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.23	J/mol×K	431.80	Joback Method
cpg	315.85	J/mol×K	461.34	Joback Method
cpg	330.80	J/mol×K	490.89	Joback Method
cpg	345.08	J/mol×K	520.43	Joback Method
cpg	358.72	J/mol×K	549.97	Joback Method
cpg	371.75	J/mol×K	579.52	Joback Method
cpg	384.19	J/mol×K	609.06	Joback Method

Sources

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=C2050819&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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