

2,6,6-trimethyl-1-heptene

Other names:	2,6,6-Trimethyl-1-heptene
Inchi:	InChI=1S/C10H20/c1-9(2)7-6-8-10(3,4)5/h1,6-8H2,2-5H3
InchiKey:	IFCGIPCIRFURCI-UHFFFAOYSA-N
Formula:	C10H20
SMILES:	C=C(C)CCCC(C)(C)C
Mol. weight [g/mol]:	140.27

Physical Properties

Property code	Value	Unit	Source
af	0.3544		Cheméo Relay (1.0)
gf	115.45	kJ/mol	Joback Method
hf	-171.83	kJ/mol	Cheméo Relay (1.0)
hfus	11.65	kJ/mol	Joback Method
hvap	44.04	kJ/mol	Cheméo Relay (1.0)
ie	9.15	eV	Cheméo Relay (1.0)
log10ws	-5.04		Cheméo Relay (1.0)
logp	3.779		Crippen Method
mcvol	147.460	ml/mol	McGowan Method
pc	2241.88	kPa	Joback Method
tb	426.67	K	Cheméo Relay (1.0)
tc	589.10	K	Cheméo Relay (1.0)
tf	208.94	K	Cheméo Relay (1.0)
vc	0.532	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.75	J/mol×K	421.53	Joback Method
cpg	317.11	J/mol×K	451.44	Joback Method
cpg	332.68	J/mol×K	481.35	Joback Method
cpg	347.47	J/mol×K	511.25	Joback Method
cpg	361.53	J/mol×K	541.16	Joback Method
cpg	374.89	J/mol×K	571.07	Joback Method
cpg	387.56	J/mol×K	600.98	Joback Method

Sources

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=T999910053&Units=SI

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
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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