2,4,6-Trimethyl-1-heptene

Other names: 1-Heptene, 2,4,6-trimethyl
Inchi: InChI=1S/C10H20/c1-8(2)6-10(5)7-9(3)4/h9-10H,1,6-7H2,2-5H3
InchiKey: HZYGXQDUQZVUFS-UHFFFAOYSA-N
Formula: C10H20
SMILES: C=C(C)CC(C)CC(C)C
Mol. weight [g/mol]: 140.27

Physical Properties

Property code	Value	Unit	Source
gf	107.73	kJ/mol	Joback Method
hf	-144.65	kJ/mol	Joback Method
hfus	12.02	kJ/mol	Joback Method
hvap	36.49	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	3.635		Crippen Method
mcvol	147.460	ml/mol	McGowan Method
pc	2235.52	kPa	Joback Method
rinpol	895.00		NIST Webbook
rinpol	895.00		NIST Webbook
rinpol	900.00		NIST Webbook
tb	423.88	K	Joback Method
tc	600.18	K	Joback Method
tf	156.74	K	Joback Method
vc	0.566	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.02	J/mol×K	423.88	Joback Method
cpg	314.72	J/mol×K	453.26	Joback Method
cpg	329.76	J/mol×K	482.65	Joback Method
cpg	344.16	J/mol×K	512.03	Joback Method
cpg	357.95	J/mol×K	541.42	Joback Method
cpg	371.14	J/mol×K	570.80	Joback Method

cpg	383.75	J/mol×K	600.18	Joback Method

Sources

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=R529636&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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