1,6-Heptadiene, 2,4,6-trimethyl

Inchi: InChI=1S/C10H18/c1-8(2)6-10(5)7-9(3)4/h10H,1,3,6-7H2,2,4-5H3
InchiKey: YYNMZKQSDYWCEJ-UHFFFAOYSA-N
Formula: C10H18
SMILES: C=C(C)CC(C)CC(=C)C
Mol. weight [g/mol]: 138.25

Physical Properties

Property code	Value	Unit	Source
gf	189.46	kJ/mol	Joback Method
hf	-23.73	kJ/mol	Joback Method
hfus	12.95	kJ/mol	Joback Method
hvap	36.29	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.555		Crippen Method
mcvol	143.160	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
rinpol	913.00		NIST Webbook
tb	420.88	K	Joback Method
tc	600.22	K	Joback Method
tf	156.02	K	Joback Method
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.00	J/mol×K	420.88	Joback Method
cpg	298.01	J/mol×K	450.77	Joback Method
cpg	312.36	J/mol×K	480.66	Joback Method
cpg	326.06	J/mol×K	510.55	Joback Method
cpg	339.13	J/mol×K	540.44	Joback Method
cpg	351.59	J/mol×K	570.33	Joback Method
cpg	363.48	J/mol×K	600.22	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=R568106&Units=SI

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