3-Heptyne, 2,2,5,5,6,6-hexamethyl

Inchi: InChI=1S/C13H24/c1-11(2,3)9-10-13(7,8)12(4,5)6/h1-8H3
InchiKey: BTMUFCOCPRKEIC-UHFFFAOYSA-N
Formula: C13H24
SMILES: CC(C)(C)C#CC(C)(C)C(C)(C)C
Mol. weight [g/mol]: 180.33

Physical Properties

Property code	Value	Unit	Source
gf	269.90	kJ/mol	Joback Method
hf	-65.60	kJ/mol	Joback Method
hfus	10.31	kJ/mol	Joback Method
hvap	42.80	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	4.108		Crippen Method
mcvol	185.430	ml/mol	McGowan Method
pc	1977.07	kPa	Joback Method
rinpol	956.00		NIST Webbook
tb	496.15	K	Joback Method
tc	711.46	K	Joback Method
tf	349.63	K	Joback Method
vc	0.693	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.73	J/mol×K	496.15	Joback Method
cpg	453.15	J/mol×K	532.04	Joback Method
cpg	473.11	J/mol×K	567.92	Joback Method
cpg	491.71	J/mol×K	603.81	Joback Method
cpg	509.03	J/mol×K	639.69	Joback Method
cpg	525.17	J/mol×K	675.58	Joback Method
cpg	540.23	J/mol×K	711.46	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=R66607&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