3-Heptyne, 2,2,5,6,6-pentamethyl

Inchi: InChI=1S/C12H22/c1-10(12(5,6)7)8-9-11(2,3)4/h10H,1-7H3
InchiKey: XRFNXAZVPMFYEM-UHFFFAOYSA-N
Formula: C12H22
SMILES: CC(C#CC(C)(C)C)C(C)(C)C
Mol. weight [g/mol]: 166.30

Physical Properties

Property code	Value	Unit	Source
gf	256.20	kJ/mol	Joback Method
hf	-41.49	kJ/mol	Joback Method
hfus	11.61	kJ/mol	Joback Method
hvap	41.48	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.718		Crippen Method
mcvol	171.340	ml/mol	McGowan Method
pc	2135.43	kPa	Joback Method
rinpol	914.00		NIST Webbook
rinpol	914.00		NIST Webbook
tb	476.06	K	Joback Method
tc	685.66	K	Joback Method
tf	320.94	K	Joback Method
vc	0.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.89	J/mol×K	476.06	Joback Method
cpg	401.63	J/mol×K	510.99	Joback Method
cpg	420.16	J/mol×K	545.93	Joback Method
cpg	437.55	J/mol×K	580.86	Joback Method
cpg	453.86	J/mol×K	615.80	Joback Method
cpg	469.16	J/mol×K	650.73	Joback Method
cpg	483.51	J/mol×K	685.66	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=R66611&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