3-Heptyne, 5-ethyl-2,2,5-trimethyl

Inchi: InChI=1S/C12H22/c1-7-12(6,8-2)10-9-11(3,4)5/h7-8H2,1-6H3
InchiKey: XJMLJFUUHRMIAY-UHFFFAOYSA-N
Formula: C12H22
SMILES: CCC(C)(C#CC(C)(C)C)CC
Mol. weight [g/mol]: 166.30

Physical Properties

Property code	Value	Unit	Source
gf	258.64	kJ/mol	Joback Method
hf	-36.21	kJ/mol	Joback Method
hfus	15.13	kJ/mol	Joback Method
hvap	41.87	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.862		Crippen Method
mcvol	171.340	ml/mol	McGowan Method
pc	2119.73	kPa	Joback Method
rinpol	906.00		NIST Webbook
rinpol	906.00		NIST Webbook
tb	476.50	K	Joback Method
tc	681.33	K	Joback Method
tf	335.94	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.79	J/mol×K	476.50	Joback Method
cpg	400.99	J/mol×K	510.64	Joback Method
cpg	419.06	J/mol×K	544.78	Joback Method
cpg	436.03	J/mol×K	578.92	Joback Method
cpg	451.99	J/mol×K	613.06	Joback Method
cpg	466.98	J/mol×K	647.20	Joback Method
cpg	481.08	J/mol×K	681.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R66657&Units=SI
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

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