

3-Ethyl-3-phenyl-1-pentene

Inchi:	InChI=1S/C13H18/c1-4-13(5-2,6-3)12-10-8-7-9-11-12/h4,7-11H,1,5-6H2,2-3H3
InchiKey:	JUYLWJTWBDJSLZ-UHFFFAOYSA-N
Formula:	C13H18
SMILES:	C=CC(CC)(CC)c1ccccc1
Mol. weight [g/mol]:	174.28
CAS:	19781-34-1

Physical Properties

Property code	Value	Unit	Source
gf	261.67	kJ/mol	Joback Method
hf	41.56	kJ/mol	Joback Method
hfus	14.77	kJ/mol	Joback Method
hvap	44.84	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.930		Crippen Method
mcvol	165.970	ml/mol	McGowan Method
pc	2324.78	kPa	Joback Method
tb	503.13 ± 0.60	K	NIST Webbook
tc	730.48	K	Joback Method
tf	263.35	K	Joback Method
vc	0.625	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.72	J/mol×K	516.97	Joback Method
cpg	395.04	J/mol×K	552.56	Joback Method
cpg	412.15	J/mol×K	588.14	Joback Method
cpg	428.11	J/mol×K	623.73	Joback Method
cpg	442.98	J/mol×K	659.31	Joback Method
cpg	456.85	J/mol×K	694.90	Joback Method
cpg	469.78	J/mol×K	730.48	Joback Method
dvisc	0.0048464	Paxs	263.35	Joback Method
dvisc	0.0019400	Paxs	305.62	Joback Method

dvisc	0.0009700	Paxs	347.89	Joback Method
dvisc	0.0005636	Paxs	390.16	Joback Method
dvisc	0.0003642	Paxs	432.43	Joback Method
dvisc	0.0002543	Paxs	474.70	Joback Method
dvisc	0.0001884	Paxs	516.97	Joback Method

Sources

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=C19781341&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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