3-Heptene, 3-ethyl-

Other names:	3-ethyl-3-heptene
Inchi:	InChI=1S/C9H18/c1-4-7-8-9(5-2)6-3/h8H,4-7H2,1-3H3
InchiKey:	VUFGUGXXEWJSBM-UHFFFAOYSA-N
Formula:	C9H18
SMILES:	CCCC=C(CC)CC
Mol. weight [g/mol]:	126.24
CAS:	74764-46-8

Physical Properties

Property code	Value	Unit	Source
gf	96.57	kJ/mol	Joback Method
hf	-121.66	kJ/mol	Joback Method
hfus	17.96	kJ/mol	Joback Method
hvap	35.67	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.533		Crippen Method
mcvol	133.370	ml/mol	McGowan Method
pc	2438.65	kPa	Joback Method
tb	409.36	K	Joback Method
tc	583.79	K	Joback Method
tf	172.15	K	Joback Method
vc	0.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.03	J/mol×K	409.36	Joback Method
cpg	272.25	J/mol×K	438.43	Joback Method
cpg	285.86	J/mol×K	467.50	Joback Method
cpg	298.88	J/mol×K	496.58	Joback Method
cpg	311.33	J/mol×K	525.65	Joback Method
cpg	323.24	J/mol×K	554.72	Joback Method
cpg	334.62	J/mol×K	583.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74764468&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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