(E)-4-Methylhept-3-ene

Other names: 3-Heptene, 4-methyl-, trans
Inchi: InChI=1S/C8H16/c1-4-6-8(3)7-5-2/h6H,4-5,7H2,1-3H3/b8-6+
InchiKey: KKVVJQGDNYIIMN-SOFGYWHQSA-N
Formula: C8H16
SMILES: CCC=C(C)CCC
Mol. weight [g/mol]: 112.21

Physical Properties

Property code	Value	Unit	Source
gf	88.15	kJ/mol	Joback Method
hf	-101.02	kJ/mol	Joback Method
hfus	15.37	kJ/mol	Joback Method
hvap	33.44	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	3.143		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2687.42	kPa	Joback Method
rinpol	791.30		NIST Webbook
rinpol	791.00		NIST Webbook
rinpol	791.00		NIST Webbook
rinpol	779.00		NIST Webbook
rinpol	778.00		NIST Webbook
rinpol	791.00		NIST Webbook
rinpol	791.30		NIST Webbook
tb	386.48	K	Joback Method
tc	561.75	K	Joback Method
tf	160.88	K	Joback Method
vc	0.465	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.03	J/mol×K	386.48	Joback Method
cpg	231.15	J/mol×K	415.69	Joback Method

cpg	243.70	J/mol×K	444.90	Joback Method
cpg	255.70	J/mol×K	474.11	Joback Method
cpg	267.18	J/mol×K	503.32	Joback Method
cpg	278.15	J/mol×K	532.54	Joback Method
cpg	288.64	J/mol×K	561.75	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R293040&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