4-Methyl-1,4-heptadiene

Inchi: InChI=1S/C8H14/c1-4-6-8(3)7-5-2/h4,7H,1,5-6H2,2-3H3/b8-7+
InchiKey: NZXFAMRCCGUQGQ-BQYQJAHWSA-N
Formula: C8H14
SMILES: C=CCC(C)=CCC
Mol. weight [g/mol]: 110.20
CAS: 13857-55-1

Physical Properties

Property code	Value	Unit	Source
gf	175.99	kJ/mol	Joback Method
hf	24.41	kJ/mol	Joback Method
hfus	14.09	kJ/mol	Joback Method
hvap	32.77	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.919		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	2808.38	kPa	Joback Method
tb	383.16	K	Joback Method
tc	562.15	K	Joback Method
tf	159.12	K	Joback Method
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.46	J/mol×K	383.16	Joback Method
cpg	216.02	J/mol×K	412.99	Joback Method
cpg	227.98	J/mol×K	442.82	Joback Method
cpg	239.38	J/mol×K	472.65	Joback Method
cpg	250.23	J/mol×K	502.48	Joback Method
cpg	260.56	J/mol×K	532.31	Joback Method
cpg	270.39	J/mol×K	562.15	Joback Method

Sources

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=C13857551&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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