2-METHYL-3-ETHYL-1,5-HEXADIENE

Inchi: InChI=1S/C8H14/c1-5-6-8(4)7(2)3/h5,8H,1-2,6H2,3-4H3
InchiKey: GRCQSGCHLQHSTC-MRVPVSSYSA-N
Formula: C8H14
SMILES: C=CCC(C)C(=C)C
Mol. weight [g/mol]: 124.22

Physical Properties

Property code	Value	Unit	Source
gf	181.17	kJ/mol	Joback Method
hf	27.34	kJ/mol	Joback Method
hfus	9.08	kJ/mol	Joback Method
hvap	31.75	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.775		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	2802.44	kPa	Joback Method
tb	375.24	K	Joback Method
tc	552.99	K	Joback Method
tf	147.44	K	Joback Method
vc	0.441	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.25	J/mol×K	375.24	Joback Method
cpg	215.79	J/mol×K	404.86	Joback Method
cpg	227.78	J/mol×K	434.49	Joback Method
cpg	239.24	J/mol×K	464.11	Joback Method
cpg	250.17	J/mol×K	493.74	Joback Method
cpg	260.61	J/mol×K	523.36	Joback Method
cpg	270.56	J/mol×K	552.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=396

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