2,4-Hexadiene, 2-ethoxy

Inchi: InChI=1S/C8H14O/c1-4-6-7-8(3)9-5-2/h4,6-7H,5H2,1-3H3/b6-4+,8-7-
InchiKey: SYZPTNQVXBBYES-AQXDOAQYSA-N
Formula: C8H14O
SMILES: CC=CC=C(C)OCC
Mol. weight [g/mol]: 126.20

Physical Properties

Property code	Value	Unit	Source
gf	63.37	kJ/mol	Joback Method
hf	-116.02	kJ/mol	Joback Method
hfus	16.76	kJ/mol	Joback Method
hvap	35.81	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.503		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	2787.66	kPa	Joback Method
rinpol	936.00		NIST Webbook
tb	413.06	K	Joback Method
tc	597.41	K	Joback Method
tf	178.03	K	Joback Method
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.58	J/mol×K	413.06	Joback Method
cpg	240.08	J/mol×K	443.78	Joback Method
cpg	252.01	J/mol×K	474.51	Joback Method
cpg	263.39	J/mol×K	505.23	Joback Method
cpg	274.24	J/mol×K	535.96	Joback Method
cpg	284.59	J/mol×K	566.68	Joback Method
cpg	294.45	J/mol×K	597.41	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R67770&Units=SI

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