E-1-Methoxy-7-methyl-1,6-octadiene

Inchi: InChI=1S/C10H18O/c1-10(2)8-6-4-5-7-9-11-3/h7-9H,4-6H2,1-3H3/b9-7+
InchiKey: ZKGWPONGWWMTFS-VQHVLOKHSA-N
Formula: C10H18O
SMILES: COC=CCCCC=C(C)C
Mol. weight [g/mol]: 154.25

Physical Properties

Property code	Value	Unit	Source
gf	80.21	kJ/mol	Joback Method
hf	-157.30	kJ/mol	Joback Method
hfus	21.94	kJ/mol	Joback Method
hvap	40.26	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.283		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2298.11	kPa	Joback Method
rinpol	1194.00		NIST Webbook
rinpol	1194.00		NIST Webbook
tb	458.82	K	Joback Method
tc	640.13	K	Joback Method
tf	200.57	K	Joback Method
vc	0.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.74	J/mol×K	458.82	Joback Method
cpg	325.32	J/mol×K	489.04	Joback Method
cpg	339.25	J/mol×K	519.26	Joback Method
cpg	352.54	J/mol×K	549.48	Joback Method
cpg	365.22	J/mol×K	579.69	Joback Method
cpg	377.32	J/mol×K	609.91	Joback Method
cpg	388.87	J/mol×K	640.13	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=R341614&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