Pentane, 3-[(1,2-dimethyl-1-propenyl)oxy]-

Inchi: InChI=1S/C10H20O/c1-6-10(7-2)11-9(5)8(3)4/h10H,6-7H2,1-5H3
InchiKey: NUIRWAXGEMRSTC-UHFFFAOYSA-N
Formula: C10H20O
SMILES: CCC(CC)OC(C)=C(C)C
Mol. weight [g/mol]: 156.27
CAS: 56798-19-7

Physical Properties

Property code	Value	Unit	Source
gf	-11.00	kJ/mol	Joback Method
hf	-289.59	kJ/mol	Joback Method
hfus	16.90	kJ/mol	Joback Method
hvap	39.99	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.505		Crippen Method
mcvol	153.330	ml/mol	McGowan Method
pc	2214.53	kPa	Joback Method
tb	454.10	K	Joback Method
tc	634.27	K	Joback Method
tf	176.69	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.61	J/mol×K	454.10	Joback Method
cpg	342.07	J/mol×K	484.13	Joback Method
cpg	356.90	J/mol×K	514.16	Joback Method
cpg	371.12	J/mol×K	544.19	Joback Method
cpg	384.73	J/mol×K	574.22	Joback Method
cpg	397.77	J/mol×K	604.25	Joback Method
cpg	410.24	J/mol×K	634.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56798197&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume