

2-(3-Pentoxy)-3-methyl-1-butene

Inchi:	InChI=1S/C10H20O/c1-6-10(7-2)11-9(5)8(3)4/h8,10H,5-7H2,1-4H3
InchiKey:	GCRGZVPKBFPEY-UHFFFAOYSA-N
Formula:	C10H20O
SMILES:	C=C(OC(CC)CC)C(C)C
Mol. weight [g/mol]:	156.27
CAS:	56798-18-6

Physical Properties

Property code	Value	Unit	Source
gf	2.73	kJ/mol	Joback Method
hf	-276.87	kJ/mol	Joback Method
hfus	13.21	kJ/mol	Joback Method
hvap	38.90	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	3.361		Crippen Method
mcvol	153.330	ml/mol	McGowan Method
pc	2200.01	kPa	Joback Method
tb	446.30	K	Joback Method
tc	622.33	K	Joback Method
tf	178.97	K	Joback Method
vc	0.584	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.59	J/mol×K	446.30	Joback Method
cpg	340.88	J/mol×K	475.64	Joback Method
cpg	355.60	J/mol×K	504.98	Joback Method
cpg	369.74	J/mol×K	534.32	Joback Method
cpg	383.32	J/mol×K	563.66	Joback Method
cpg	396.34	J/mol×K	592.99	Joback Method
cpg	408.83	J/mol×K	622.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56798186&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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