1-(3-Methyl-2-butenoxy)-4-(1-propenyl)benzene

Other names: Benzene, 1-(3-methyl-2-butenoxy)-4-(1-propenyl)-
foeniculin
Inchi: InChI=1S/C14H18O/c1-4-5-13-6-8-14(9-7-13)15-11-10-12(2)3/h4-10H,11H2,1-3H3/b5-4+
InchiKey: JGELFJUQMIUNOO-SNAWJCMRSA-N
Formula: C14H18O
SMILES: CC=Cc1ccc(OCC=C(C)C)cc1
Mol. weight [g/mol]: 202.29
CAS: 78259-41-3

Physical Properties

Property code	Value	Unit	Source
gf	216.67	kJ/mol	Joback Method
hf	-14.80	kJ/mol	Joback Method
hfus	25.95	kJ/mol	Joback Method
hvap	52.10	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	4.065		Crippen Method
mcvol	181.630	ml/mol	McGowan Method
pc	2155.30	kPa	Joback Method
rinpol	1684.00		NIST Webbook
rinpol	1684.00		NIST Webbook
tb	582.00	K	Joback Method
tc	796.02	K	Joback Method
tf	284.59	K	Joback Method
vc	0.691	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.47	J/mol×K	582.00	Joback Method
cpg	448.34	J/mol×K	617.67	Joback Method
cpg	464.21	J/mol×K	653.34	Joback Method
cpg	479.13	J/mol×K	689.01	Joback Method
cpg	493.15	J/mol×K	724.68	Joback Method

cpg	506.33	J/mol×K	760.35	Joback Method
cpg	518.72	J/mol×K	796.02	Joback Method

Sources

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=C78259413&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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