Oxetane, 3-methyl-3-phenoxymethyl

Inchi: InChI=1S/C11H14O2/c1-11(7-12-8-11)9-13-10-5-3-2-4-6-10/h2-6H,7-9H2,1H3
InchiKey: DMVWICDWJIUWPO-UHFFFAOYSA-N
Formula: C11H14O2
SMILES: CC1(COc2ccccc2)COC1
Mol. weight [g/mol]: 178.23

Physical Properties

Property code	Value	Unit	Source
gf	6.19	kJ/mol	Joback Method
hf	-216.18	kJ/mol	Joback Method
hfus	17.19	kJ/mol	Joback Method
hvap	48.21	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	2.102		Crippen Method
mcvol	142.970	ml/mol	McGowan Method
pc	3195.54	kPa	Joback Method
rinpol	1450.00		NIST Webbook
tb	538.38	K	Joback Method
tc	770.34	K	Joback Method
tf	327.27	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.16	J/mol×K	538.38	Joback Method
cpg	358.86	J/mol×K	577.04	Joback Method
cpg	374.33	J/mol×K	615.70	Joback Method
cpg	388.72	J/mol×K	654.36	Joback Method
cpg	402.21	J/mol×K	693.02	Joback Method
cpg	414.94	J/mol×K	731.68	Joback Method
cpg	427.06	J/mol×K	770.34	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=R6832&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