Oxetane, 3-methyl-3-(2-methyl-1-[3-methylphenyloxy)propy

Inchi: InChI=1S/C15H22O2/c1-11(2)14(15(4)9-16-10-15)17-13-7-5-6-12(3)8-13/h5-8,11,14H,9-

InchiKey: CVQOPSMFHSOTRA-UHFFFAOYSA-N

Formula: C15H22O2

SMILES: Cc1cccc(OC(C(C)C)C2(C)COC2)c1

Mol. weight [g/mol]: 234.33

Physical Properties

Property code	Value	Unit	Source
gf	25.36	kJ/mol	Joback Method
hf	-320.77	kJ/mol	Joback Method
hfus	20.12	kJ/mol	Joback Method
hvap	57.00	kJ/mol	Joback Method
log10ws	-3.61		Crippen Method
logp	3.435		Crippen Method
mcvol	199.330	ml/mol	McGowan Method
pc	2159.31	kPa	Joback Method
rinpol	1654.00		NIST Webbook
rinpol	1654.00		NIST Webbook
tb	634.00	K	Joback Method
tc	859.32	K	Joback Method
tf	354.87	K	Joback Method
vc	0.742	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.72	J/mol×K	634.00	Joback Method
cpg	561.11	J/mol×K	671.55	Joback Method
cpg	579.38	J/mol×K	709.11	Joback Method
cpg	596.69	J/mol×K	746.66	Joback Method
cpg	613.17	J/mol×K	784.22	Joback Method
cpg	629.00	J/mol×K	821.77	Joback Method
cpg	644.30	J/mol×K	859.32	Joback Method

Sources

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=R6816&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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