Oxetane, 3-bromomethyl-3-(4-methylphenyloxy)methyl

Inchi: InChI=1S/C12H15BrO2/c1-10-2-4-11(5-3-10)15-9-12(6-13)7-14-8-12/h2-5H,6-9H2,1H3

InchiKey: SOSJWBCYCPPDLJ-UHFFFAOYSA-N

Formula: C12H15BrO2

SMILES: Cc1ccc(OCC2(CBr)COC2)cc1

Mol. weight [g/mol]: 271.15

Physical Properties

Property code	Value	Unit	Source
gf	19.30	kJ/mol	Joback Method
hf	-221.96	kJ/mol	Joback Method
hfus	24.68	kJ/mol	Joback Method
hvap	57.53	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.785		Crippen Method
mcvol	174.560	ml/mol	McGowan Method
pc	3049.04	kPa	Joback Method
rinpol	1812.00		NIST Webbook
rinpol	1812.00		NIST Webbook
tb	632.40	K	Joback Method
tc	873.82	K	Joback Method
tf	410.86	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.69	J/mol×K	632.40	Joback Method
cpg	446.19	J/mol×K	672.64	Joback Method
cpg	460.73	J/mol×K	712.87	Joback Method
cpg	474.49	J/mol×K	753.11	Joback Method
cpg	487.66	J/mol×K	793.35	Joback Method
cpg	500.41	J/mol×K	833.58	Joback Method
cpg	512.94	J/mol×K	873.82	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R6625&Units=SI

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