Oxetane, 3-bromomethyl-3-[2-methyl-1-(3-methylphenyloxy

Inchi: InChI=1S/C15H21BrO2/c1-11(2)14(15(8-16)9-17-10-15)18-13-6-4-5-12(3)7-13/h4-7,11,1

InchiKey: JEDKQECCXUMCPK-UHFFFAOYSA-N

Formula: C15H21BrO2

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

Mol. weight [g/mol]: 313.23

Physical Properties

Property code	Value	Unit	Source
gf	39.68	kJ/mol	Joback Method
hf	-294.44	kJ/mol	Joback Method
hfus	25.40	kJ/mol	Joback Method
hvap	63.44	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.810		Crippen Method
mcvol	216.830	ml/mol	McGowan Method
pc	2304.74	kPa	Joback Method
rinpol	1943.00		NIST Webbook
tb	700.16	K	Joback Method
tc	936.50	K	Joback Method
tf	414.67	K	Joback Method
vc	0.803	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	586.75	J/mol×K	700.16	Joback Method
cpg	604.64	J/mol×K	739.55	Joback Method
cpg	621.63	J/mol×K	778.94	Joback Method
cpg	637.88	J/mol×K	818.33	Joback Method
cpg	653.58	J/mol×K	857.72	Joback Method
cpg	668.93	J/mol×K	897.11	Joback Method
cpg	684.09	J/mol×K	936.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R6612&Units=SI
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

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