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

Inchi: InChI=1S/C12H16O2/c1-10-3-5-11(6-4-10)14-9-12(2)7-13-8-12/h3-6H,7-9H2,1-2H3
InchiKey: HMSIDZYEQAXKCE-UHFFFAOYSA-N
Formula: C12H16O2
SMILES: Cc1ccc(OCC2(C)COC2)cc1
Mol. weight [g/mol]: 192.25

Physical Properties

Property code	Value	Unit	Source
gf	4.98	kJ/mol	Joback Method
hf	-248.29	kJ/mol	Joback Method
hfus	19.39	kJ/mol	Joback Method
hvap	51.10	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.410		Crippen Method
mcvol	157.060	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
rinpol	1528.00		NIST Webbook
tb	566.24	K	Joback Method
tc	794.89	K	Joback Method
tf	351.06	K	Joback Method
vc	0.586	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.52	J/mol×K	566.24	Joback Method
cpg	406.50	J/mol×K	604.35	Joback Method
cpg	422.38	J/mol×K	642.46	Joback Method
cpg	437.28	J/mol×K	680.57	Joback Method
cpg	451.35	J/mol×K	718.67	Joback Method
cpg	464.75	J/mol×K	756.78	Joback Method
cpg	477.60	J/mol×K	794.89	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=R6829&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