epoxytagetone

Inchi: InChI=1S/C10H16O2/c1-5-10(4)9(12-10)8(11)6-7(2)3/h5,7,9H,1,6H2,2-4H3
InchiKey: ZWTQFBZSHCNGGC-UHFFFAOYSA-N
Formula: C10H16O2
SMILES: C=CC1(C)OC1C(=O)CC(C)C
Mol. weight [g/mol]: 168.23

Physical Properties

Property code	Value	Unit	Source
gf	-48.77	kJ/mol	Joback Method
hf	-306.46	kJ/mol	Joback Method
hfus	19.34	kJ/mol	Joback Method
hvap	46.51	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	1.945		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
ripol	1696.00		NIST Webbook
ripol	1696.00		NIST Webbook
tb	507.57	K	Joback Method
tc	708.27	K	Joback Method
tf	299.80	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.31	J/mol×K	507.57	Joback Method
cpg	357.29	J/mol×K	541.02	Joback Method
cpg	371.29	J/mol×K	574.47	Joback Method
cpg	384.41	J/mol×K	607.92	Joback Method
cpg	396.77	J/mol×K	641.37	Joback Method
cpg	408.47	J/mol×K	674.82	Joback Method
cpg	419.61	J/mol×K	708.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R315927&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume