isololiolide

Inchi: InChI=1S/C11H16O3/c1-10(2)5-7(12)6-11(3)8(10)4-9(13)14-11/h4,7,12H,5-6H2,1-3H3/t7
InchiKey: XEVQXKKKAVVSMW-HQJQHLMTSA-N
Formula: C11H16O3
SMILES: CC1(C)CC(O)CC2(C)OC(=O)C=C12
Mol. weight [g/mol]: 196.24

Physical Properties

Property code	Value	Unit	Source
gf	-216.95	kJ/mol	Joback Method
hf	-508.73	kJ/mol	Joback Method
hfus	15.10	kJ/mol	Joback Method
hvap	64.20	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	1.409		Crippen Method
mcvol	153.140	ml/mol	McGowan Method
pc	3291.59	kPa	Joback Method
ripol	3228.00		NIST Webbook
ripol	3228.00		NIST Webbook
tb	664.27	K	Joback Method
tc	889.62	K	Joback Method
tf	451.50	K	Joback Method
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.58	J/mol×K	664.27	Joback Method
cpg	457.59	J/mol×K	701.83	Joback Method
cpg	472.08	J/mol×K	739.39	Joback Method
cpg	486.28	J/mol×K	776.95	Joback Method
cpg	500.39	J/mol×K	814.51	Joback Method
cpg	514.62	J/mol×K	852.06	Joback Method
cpg	529.19	J/mol×K	889.62	Joback Method

Sources

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=R399356&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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