Methyl 2,3-di-epi-cucurbate

Inchi: InChI=1S/C13H22O3/c1-3-4-5-6-11-10(7-8-12(11)14)9-13(15)16-2/h4-5,10-12,14H,3,6-9
InchiKey: OOYCGMQJIWHWHA-IUOCUSHJSA-N
Formula: C13H22O3
SMILES: CCC=CCC1C(O)CCC1CC(=O)OC
Mol. weight [g/mol]: 226.31

Physical Properties

Property code	Value	Unit	Source
gf	-210.81	kJ/mol	Joback Method
hf	-571.66	kJ/mol	Joback Method
hfus	32.58	kJ/mol	Joback Method
hvap	69.96	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	2.293		Crippen Method
mcvol	192.180	ml/mol	McGowan Method
pc	2139.38	kPa	Joback Method
rinpol	1636.00		NIST Webbook
tb	675.41	K	Joback Method
tc	863.59	K	Joback Method
tf	366.59	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.89	J/mol×K	675.41	Joback Method
cpg	571.77	J/mol×K	706.77	Joback Method
cpg	586.80	J/mol×K	738.14	Joback Method
cpg	601.00	J/mol×K	769.50	Joback Method
cpg	614.40	J/mol×K	800.86	Joback Method
cpg	627.02	J/mol×K	832.22	Joback Method
cpg	638.89	J/mol×K	863.59	Joback Method
dvisc	0.0033029	Pa×s	366.59	Joback Method
dvisc	0.0012003	Pa×s	418.06	Joback Method

dvisc	0.0005445	Pa×s	469.53	Joback Method
dvisc	0.0002888	Pa×s	521.00	Joback Method
dvisc	0.0001717	Pa×s	572.47	Joback Method
dvisc	0.0001112	Pa×s	623.94	Joback Method
dvisc	0.0000769	Pa×s	675.41	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=R233820&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
dvisc:	Dynamic viscosity
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