flourensadiol

Inchi: InChI=1S/C16H28O/c1-10-5-6-11-13(10)14-12(16(14,4)9-17)7-8-15(11,2)3/h10-14,17H,5
InchiKey: LTVWWYLRQMIEHW-ISXYAVKNSA-N
Formula: C16H28O
SMILES: CC1CCC2C1C1C(CCC2(C)C)C1(C)CO
Mol. weight [g/mol]: 236.39
CAS: 55812-89-0

Physical Properties

Property code	Value	Unit	Source
gf	63.25	kJ/mol	Joback Method
hf	-370.60	kJ/mol	Joback Method
hfus	23.18	kJ/mol	Joback Method
hvap	64.43	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.713		Crippen Method
mcvol	209.590	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
rinpol	1864.00		NIST Webbook
tb	668.22	K	Joback Method
tc	871.48	K	Joback Method
tf	408.52	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.19	J/mol×K	668.22	Joback Method
cpg	677.05	J/mol×K	702.10	Joback Method
cpg	697.05	J/mol×K	735.97	Joback Method
cpg	716.41	J/mol×K	769.85	Joback Method
cpg	735.35	J/mol×K	803.73	Joback Method
cpg	754.07	J/mol×K	837.60	Joback Method
cpg	772.79	J/mol×K	871.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55812890&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