Methyl-2«alpha»-[2'(m-isopropylphenyl)ethyl]-1«b

Inchi: InChI=1S/C21H32O2/c1-15(2)18-9-6-10-19(12-18)17(4)14-23-20(22)21(5)11-7-8-16(3)13
InchiKey: WXKLQRUTMXPCIA-XGHQBKJUSA-N
Formula: C21H32O2
SMILES: CC1CCCC(C)(C(=O)OCC(C)c2cccc(C(C)C)c2)C1
Mol. weight [g/mol]: 316.48

Physical Properties

Property code	Value	Unit	Source
gf	1.17	kJ/mol	Joback Method
hf	-457.85	kJ/mol	Joback Method
hfus	26.15	kJ/mol	Joback Method
hvap	72.63	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	5.673		Crippen Method
mcvol	279.570	ml/mol	McGowan Method
pc	1435.89	kPa	Joback Method
rinpol	2130.00		NIST Webbook
tb	802.07	K	Joback Method
tc	1026.22	K	Joback Method
tf	434.57	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	881.25	J/mol×K	802.07	Joback Method
cpg	903.47	J/mol×K	839.43	Joback Method
cpg	924.64	J/mol×K	876.79	Joback Method
cpg	944.91	J/mol×K	914.15	Joback Method
cpg	964.41	J/mol×K	951.51	Joback Method
cpg	983.30	J/mol×K	988.86	Joback Method
cpg	1001.71	J/mol×K	1026.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R149418&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume