10-epi-Italicen-12-yl 2-methylbutyrate

Inchi: InChI=1S/C20H32O2/c1-6-14(3)18(21)22-12-19(5)16-8-7-15(4)20(16)10-9-13(2)11-17(19
InchiKey: UBHUQRYYLLGBFL-VIVDETTOSA-N
Formula: C20H32O2
SMILES: CCC(C)C(=O)OCC1(C)C2C=C(C)CCC23C(C)CCC13
Mol. weight [g/mol]: 304.47

Physical Properties

Property code	Value	Unit	Source
gf	33.14	kJ/mol	Joback Method
hf	-464.02	kJ/mol	Joback Method
hfus	27.40	kJ/mol	Joback Method
hvap	67.00	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	4.984		Crippen Method
mcvol	263.220	ml/mol	McGowan Method
pc	1480.43	kPa	Joback Method
rinpol	2000.00		NIST Webbook
rinpol	2000.00		NIST Webbook
tb	756.89	K	Joback Method
tc	972.13	K	Joback Method
tf	471.70	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	842.97	J/mol×K	756.89	Joback Method
cpg	865.76	J/mol×K	792.76	Joback Method
cpg	888.05	J/mol×K	828.64	Joback Method
cpg	910.10	J/mol×K	864.51	Joback Method
cpg	932.16	J/mol×K	900.39	Joback Method
cpg	954.49	J/mol×K	936.26	Joback Method
cpg	977.34	J/mol×K	972.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R232976&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