15-Keto-PGD2 TMS

Inchi: InChI=1S/C20H30O5/c1-2-3-6-9-15(21)12-13-17-16(18(22)14-19(17)23)10-7-4-5-8-11-20
InchiKey: XEQAHADLFLAPQL-AQDJLICYSA-N
Formula: C20H30O5
SMILES: CCCCCC(=O)C=CC1C(=O)CC(O)C1CC=CCCCC(=O)O
Mol. weight [g/mol]: 350.45

Physical Properties

Property code	Value	Unit	Source
gf	-354.98	kJ/mol	Joback Method
hf	-869.21	kJ/mol	Joback Method
hfus	54.92	kJ/mol	Joback Method
hvap	110.77	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	3.459		Crippen Method
mcvol	289.650	ml/mol	McGowan Method
pc	1508.15	kPa	Joback Method
rinpol	2827.00		NIST Webbook
tb	1031.18	K	Joback Method
tc	1264.20	K	Joback Method
tf	597.14	K	Joback Method
vc	1.111	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1012.85	J/mol×K	1031.18	Joback Method
cpg	1026.30	J/mol×K	1070.02	Joback Method
cpg	1038.53	J/mol×K	1108.85	Joback Method
cpg	1049.60	J/mol×K	1147.69	Joback Method
cpg	1059.57	J/mol×K	1186.53	Joback Method
cpg	1068.51	J/mol×K	1225.36	Joback Method
cpg	1076.50	J/mol×K	1264.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R16769&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