

Santamarine

Inchi:	InChI=1S/C15H20O3/c1-8-4-5-11(16)15(3)7-6-10-9(2)14(17)18-13(10)12(8)15/h4,10-13,
InchiKey:	PLSSEPIRACGCBO-UHFFFAOYSA-N
Formula:	C15H20O3
SMILES:	C=C1C(=O)OC2C1CCC1(C)C(O)CC=C(C)C21
Mol. weight [g/mol]:	248.32
CAS:	4290-13-5

Physical Properties

Property code	Value	Unit	Source
gf	-83.76	kJ/mol	Joback Method
hf	-475.99	kJ/mol	Joback Method
hfus	27.71	kJ/mol	Joback Method
hvap	74.19	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	2.211		Crippen Method
mcvol	194.340	ml/mol	McGowan Method
pc	2424.27	kPa	Joback Method
rinpol	2227.00		NIST Webbook
rinpol	2227.00		NIST Webbook
tb	761.05	K	Joback Method
tc	985.40	K	Joback Method
tf	496.54	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	626.84	J/molxK	761.05	Joback Method
cpg	644.68	J/molxK	798.44	Joback Method
cpg	661.77	J/molxK	835.83	Joback Method
cpg	678.24	J/molxK	873.22	Joback Method
cpg	694.23	J/molxK	910.62	Joback Method
cpg	709.85	J/molxK	948.01	Joback Method
cpg	725.26	J/molxK	985.40	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4290135&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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