Reynosin

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/h10-13,16
InchiKey: FKBUODICGDOIGB-UHFFFAOYSA-N
Formula: C15H20O3
SMILES: C=C1C(=O)OC2C1CCC1(C)C(O)CCC(=C)C21
Mol. weight [g/mol]: 248.32
CAS: 28254-53-7

Physical Properties

Property code	Value	Unit	Source
gf	-51.01	kJ/mol	Joback Method
hf	-438.06	kJ/mol	Joback Method
hfus	25.71	kJ/mol	Joback Method
hvap	73.40	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	2.211		Crippen Method
mcvol	194.340	ml/mol	McGowan Method
pc	2419.50	kPa	Joback Method
rinpol	2266.10		NIST Webbook
rinpol	2266.10		NIST Webbook
tb	756.07	K	Joback Method
tc	979.49	K	Joback Method
tf	496.94	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	626.67	J/mol×K	756.07	Joback Method
cpg	644.65	J/mol×K	793.31	Joback Method
cpg	661.84	J/mol×K	830.54	Joback Method
cpg	678.37	J/mol×K	867.78	Joback Method
cpg	694.37	J/mol×K	905.01	Joback Method
cpg	709.96	J/mol×K	942.25	Joback Method
cpg	725.29	J/mol×K	979.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28254537&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