Hydrocortamate

Inchi: InChI=1S/C27H41NO6/c1-5-28(6-2)15-23(32)34-16-22(31)27(33)12-10-20-19-8-7-17-13-
InchiKey: FWFVLWGEFDIZMJ-UHFFFAOYSA-N
Formula: C27H41NO6
SMILES: CCN(CC)CC(=O)OCC(=O)C1(O)CCC2C3CCC4=CC(=O)CCC4(C)C3C(O)CC21C
Mol. weight [g/mol]: 475.62
CAS: 76-47-1

Physical Properties

Property code	Value	Unit	Source
gf	-308.60	kJ/mol	Joback Method
hf	-1041.21	kJ/mol	Joback Method
hfus	47.97	kJ/mol	Joback Method
hvap	128.33	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	2.674		Crippen Method
mcvol	375.850	ml/mol	McGowan Method
pc	1292.07	kPa	Joback Method
tb	1251.10	K	Joback Method
tc	1546.94	K	Joback Method
tf	864.89	K	Joback Method
vc	1.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1693.24	J/mol×K	1251.10	Joback Method
cpg	1763.38	J/mol×K	1300.41	Joback Method
cpg	1840.94	J/mol×K	1349.71	Joback Method
cpg	1926.78	J/mol×K	1399.02	Joback Method
cpg	2021.78	J/mol×K	1448.32	Joback Method
cpg	2126.81	J/mol×K	1497.63	Joback Method
cpg	2242.76	J/mol×K	1546.94	Joback Method

Sources

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=C76471&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume