Rociverine

Inchi: InChI=1S/C20H37NO3/c1-4-21(5-2)15-16(3)24-19(22)18-13-9-10-14-20(18,23)17-11-7-6
InchiKey: XPYLKZZOBVLVHB-OUNSHVDWSA-N
Formula: C20H37NO3
SMILES: CCN(CC)CC(C)OC(=O)C1CCCCC1(O)C1CCCCC1
Mol. weight [g/mol]: 339.51
CAS: 53716-44-2

Physical Properties

Property code	Value	Unit	Source
gf	-109.18	kJ/mol	Joback Method
hf	-687.37	kJ/mol	Joback Method
hfus	32.37	kJ/mol	Joback Method
hvap	87.00	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	3.762		Crippen Method
mcvol	294.230	ml/mol	McGowan Method
pc	1511.67	kPa	Joback Method
rinpol	2237.00		NIST Webbook
tb	872.14	K	Joback Method
tc	1081.71	K	Joback Method
tf	500.03	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1026.01	J/mol×K	872.14	Joback Method
cpg	1047.32	J/mol×K	907.07	Joback Method
cpg	1067.74	J/mol×K	942.00	Joback Method
cpg	1087.41	J/mol×K	976.93	Joback Method
cpg	1106.44	J/mol×K	1011.85	Joback Method
cpg	1124.97	J/mol×K	1046.78	Joback Method
cpg	1143.13	J/mol×K	1081.71	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53716442&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
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