

GA11, Me

Inchi: InChI=1S/C20H24O5/c1-9-6-19-7-10(9)4-5-12(19)20-14(13(19)16(21)23-3)18(2)8-11(15)
InchiKey: NGYXRKRMVHSLN-NGMLVCFKSA-N
Formula: C20H24O5
SMILES: C=C1CC23CC1CCC2C12OC1C1CC(C)(C(=O)O1)C2C3C(=O)OC
Mol. weight [g/mol]: 344.40

Physical Properties

Property code	Value	Unit	Source
gf	-33.25	kJ/mol	Joback Method
hf	-596.89	kJ/mol	Joback Method
hfus	37.78	kJ/mol	Joback Method
hvap	77.79	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	2.241		Crippen Method
mcvol	243.950	ml/mol	McGowan Method
pc	1992.98	kPa	Joback Method
rinpol	2402.00		NIST Webbook
rinpol	2402.00		NIST Webbook
tb	881.32	K	Joback Method
tc	1128.93	K	Joback Method
tf	688.98	K	Joback Method
vc	0.946	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	900.47	J/mol×K	881.32	Joback Method
cpg	927.98	J/mol×K	922.59	Joback Method
cpg	957.44	J/mol×K	963.86	Joback Method
cpg	989.46	J/mol×K	1005.13	Joback Method
cpg	1024.62	J/mol×K	1046.39	Joback Method
cpg	1063.53	J/mol×K	1087.66	Joback Method
cpg	1106.78	J/mol×K	1128.93	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=R79195&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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