Actinodaphnine

Inchi:	InChI=1S/C18H17NO4/c1-21-14-7-11-10(5-13(14)20)4-12-16-9(2-3-19-12)6-15-18(17(11
InchiKey:	VYJUHRAQPIBWNV-UHFFFAOYSA-N
Formula:	C18H17NO4
SMILES:	COc1cc2c(cc1O)CC1NCCc3cc4c(c-2c31)OCO4
Mol. weight [g/mol]:	311.33
CAS:	517-69-1

Physical Properties

Property code	Value	Unit	Source
gf	133.34	kJ/mol	Joback Method
hf	-281.09	kJ/mol	Joback Method
hfus	55.01	kJ/mol	Joback Method
hvap	95.57	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	2.539		Crippen Method
mcvol	217.840	ml/mol	McGowan Method
pc	3072.75	kPa	Joback Method
rinpol	3108.10		NIST Webbook
rinpol	3108.10		NIST Webbook
tb	925.26	K	Joback Method
tc	1184.87	K	Joback Method
tf	778.52	K	Joback Method
vc	0.771	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	701.48	J/mol×K	925.26	Joback Method
cpg	716.81	J/mol×K	968.53	Joback Method
cpg	732.18	J/mol×K	1011.80	Joback Method
cpg	747.85	J/mol×K	1055.06	Joback Method
cpg	764.06	J/mol×K	1098.33	Joback Method
cpg	781.06	J/mol×K	1141.60	Joback Method
cpg	799.12	J/mol×K	1184.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C517691&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

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