

Shinflavanone

Inchi:	InChI=1S/C25H26O4/c1-15(2)5-6-16-13-17(7-9-20(16)26)23-14-21(27)18-8-10-22-19(24)
InchiKey:	NEIURIYDQMKXIG-UHFFFAOYSA-N
Formula:	C25H26O4
SMILES:	<chem>CC(C)=CCc1cc(C2CC(=O)c3ccc4c(c3O2)C=CC(C)(C)O4)ccc1O</chem>
Mol. weight [g/mol]:	390.47
CAS:	157414-03-4

Physical Properties

Property code	Value	Unit	Source
gf	89.91	kJ/mol	Joback Method
hf	-397.43	kJ/mol	Joback Method
hfus	54.17	kJ/mol	Joback Method
hvap	104.07	kJ/mol	Joback Method
log10ws	-7.47		Crippen Method
logp	5.792		Crippen Method
mvol	304.450	ml/mol	McGowan Method
pc	1733.22	kPa	Joback Method
rinpol	3328.90		NIST Webbook
rinpol	3328.90		NIST Webbook
tb	1072.48	K	Joback Method
tc	1339.34	K	Joback Method
tf	741.97	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1069.95	J/molxK	1072.48	Joback Method
cpg	1096.62	J/molxK	1116.96	Joback Method
cpg	1124.80	J/molxK	1161.43	Joback Method
cpg	1154.87	J/molxK	1205.91	Joback Method
cpg	1187.20	J/molxK	1250.39	Joback Method
cpg	1222.20	J/molxK	1294.86	Joback Method
cpg	1260.24	J/molxK	1339.34	Joback Method

Sources

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=C157414034&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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