

Senecivernine

Inchi:

YLF5VIMMRPNPFK-BJRXWDRESA-N

InchiKey:

YLFSVIMMRPNPFK-BJRXWDRESA-N

Formula:

C26H21F6NO5

SMILES:

CC1(C)C(C=CC(=O)OC(C(F)(F)F)C(F)(F)F)C1C(=O)OC(C#N)c1cccc(Oc2ccccc2)c1

Mol. weight [g/mol]:

541.44

CAS:

72755-25-0

Physical Properties

Property code	Value	Unit	Source
gf	-1104.43	kJ/mol	Joback Method
hf	-1615.46	kJ/mol	Joback Method
hfus	49.84	kJ/mol	Joback Method
hvap	99.72	kJ/mol	Joback Method
log10ws	-7.44		Crippen Method
logp	6.452		Crippen Method
mcvol	347.270	ml/mol	McGowan Method
pc	1059.64	kPa	Joback Method
rinpol	2331.00		NIST Webbook
rinpol	2299.00		NIST Webbook
rinpol	2285.00		NIST Webbook
rinpol	2330.00		NIST Webbook
rinpol	2303.00		NIST Webbook
rinpol	2330.00		NIST Webbook
rinpol	2299.00		NIST Webbook
rinpol	2330.00		NIST Webbook
tb	1119.78	K	Joback Method
tc	1370.98	K	Joback Method
tf	686.34	K	Joback Method
vc	1.375	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1203.87	J/mol×K	1119.78	Joback Method

cpg	1224.74	J/mol×K	1161.65	Joback Method
cpg	1246.59	J/mol×K	1203.51	Joback Method
cpg	1269.74	J/mol×K	1245.38	Joback Method
cpg	1294.49	J/mol×K	1287.25	Joback Method
cpg	1321.16	J/mol×K	1329.11	Joback Method
cpg	1350.04	J/mol×K	1370.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72755250&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
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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