Neosolaniol

Other names:	Neozolaniol Solaniol (sesquiterpene) Solaniol Trichothec-9-ene-3,4,8,15-tetrol, 12,13-epoxy-, 4,15-diacetate, (3«alpha»,4«beta»,8«alpha»)- Trichothec-9-ene-3,4,8,15-tetrol, 12,13-epoxy-, 4,15-diacetate Trichothec-9-ene-3-«alpha»,4-«beta»,8-«alpha»,15-tetrol, 12,13-epoxy-, 4,15-diacetate 4'-«beta»,15-Diacetoxy-3-«alpha»,8-«alpha»-dihydroxy-12,13-epoxytrichothec-9-ene Trichothec-9-ene, 12,13-epoxy-4-«beta»,15-diacetoxy-3-«alpha»,8-«alpha»-dihydroxy- NSC 197212
Inchi:	InChI=1S/C19H26O8/c1-9-5-13-18(6-12(9)22,7-24-10(2)20)17(4)15(26-11(3)21)14(23)16
InchiKey:	TVZHDVCTOCZDNE-MGIQOYISSA-N
Formula:	C19H26O8
SMILES:	CC(=O)OCC12CC(O)C(C)=CC1OC1C(O)C(OC(C)=O)C2(C)C12CO2
Mol. weight [g/mol]:	382.40
CAS:	36519-25-2

Physical Properties

Property code	Value	Unit	Source
gf	-612.80	kJ/mol	Joback Method
hf	-1204.00	kJ/mol	Joback Method
hfus	49.24	kJ/mol	Joback Method
hvap	114.84	kJ/mol	Joback Method
log10ws	-1.82		Crippen Method
logp	0.096		Crippen Method
mcvol	269.190	ml/mol	McGowan Method
pc	2085.03	kPa	Joback Method
rinpol	2652.00		NIST Webbook
tb	1046.64	K	Joback Method
tc	1281.68	K	Joback Method
tf	755.73	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1064.54	J/mol×K	1046.64	Joback Method
cpg	1098.28	J/mol×K	1085.81	Joback Method
cpg	1135.09	J/mol×K	1124.99	Joback Method
cpg	1175.40	J/mol×K	1164.16	Joback Method
cpg	1219.63	J/mol×K	1203.33	Joback Method
cpg	1268.21	J/mol×K	1242.50	Joback Method
cpg	1321.58	J/mol×K	1281.68	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=C36519252&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

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