

neryl 6-O-(«beta»-D-apiofuranosyl)-«beta»-D-glucopyranose

TEFA

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C33H30F18O16/c1-12(2)5-4-6-13(3)7-8-58-19-17(65-24(55)31(43,44)45)16(64)23-22-21-20-18-15-14-13-12-11-10-9-8-7-6-5-4-3-2-1

JDKOMIBOSXQNFU-NVRVFREMSA-N

C33H30F18O16

CC(C)=CCCC(C)=CCOC1OC(COC2OCC(COC(=O)C(F)(F)F)(OC(=O)C(F)(F)F)C2OC(=O)C(F)(F)F)C1

1024.55

Physical Properties

Property code	Value	Unit	Source
gf	-4895.73	kJ/mol	Joback Method
hf	-6081.31	kJ/mol	Joback Method
hfus	110.92	kJ/mol	Joback Method
hvap	133.10	kJ/mol	Joback Method
log10ws	-8.52		Crippen Method
logp	5.640		Crippen Method
mcvol	545.490	ml/mol	McGowan Method
pc	491.20	kPa	Joback Method
rinpol	2213.00		NIST Webbook
tb	1493.53	K	Joback Method
tc	2347.96	K	Joback Method
tf	996.03	K	Joback Method
vc	2.192	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2158.48	J/mol×K	1493.53	Joback Method
cpg	2237.82	J/mol×K	1635.94	Joback Method
cpg	2345.02	J/mol×K	1778.34	Joback Method
cpg	2491.85	J/mol×K	1920.75	Joback Method
cpg	2690.12	J/mol×K	2063.15	Joback Method
cpg	2951.59	J/mol×K	2205.56	Joback Method
cpg	3288.04	J/mol×K	2347.96	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=R438738&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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