

neryl «beta»-D-glucopyranoside, TFA

Inchi:	InChI=1S/C24H24F12O10/c1-10(2)5-4-6-11(3)7-8-41-16-15(46-20(40)24(34,35)36)14(45
InchiKey:	UCMHRJFXWFCWDN-ARIBZMOSSA-N
Formula:	C24H24F12O10
SMILES:	CC(C)=CCCC(C)=CCOC1OC(COC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F
Mol. weight [g/mol]:	700.42

Physical Properties

Property code	Value	Unit	Source
gf	-3165.01	kJ/mol	Joback Method
hf	-3982.61	kJ/mol	Joback Method
hfus	79.44	kJ/mol	Joback Method
hvap	96.84	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	4.948		Crippen Method
mvol	392.300	ml/mol	McGowan Method
pc	754.33	kPa	Joback Method
rinpol	1853.00		NIST Webbook
rinpol	1853.00		NIST Webbook
tb	1090.32	K	Joback Method
tc	1373.40	K	Joback Method
tf	666.78	K	Joback Method
vc	1.577	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1394.13	J/molxK	1090.32	Joback Method
cpg	1404.97	J/molxK	1137.50	Joback Method
cpg	1413.53	J/molxK	1184.68	Joback Method
cpg	1420.01	J/molxK	1231.86	Joback Method
cpg	1424.60	J/molxK	1279.04	Joback Method
cpg	1427.49	J/molxK	1326.22	Joback Method
cpg	1428.88	J/molxK	1373.40	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R438723&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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