

Nerol, Gly, TFA

Inchi:	InChI=1S/C24H24F12O10/c1-11(2)8-6-4-3-5-7-9-41-16-15(46-20(40)24(34,35)36)14(45-
InchiKey:	JNKMQSBZJOYRQZ-VLQFCQKHSA-N
Formula:	C ₂₄ H ₂₄ F ₁₂ O ₁₀
SMILES:	<chem>CC(C)=CCCCC=CCOC1OC(COC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)</chem>
Mol. weight [g/mol]:	700.42

Physical Properties

Property code	Value	Unit	Source
gf	-3156.46	kJ/mol	Joback Method
hf	-3972.82	kJ/mol	Joback Method
hfus	80.75	kJ/mol	Joback Method
hvap	96.76	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	4.948		Crippen Method
mcvol	392.300	ml/mol	McGowan Method
pc	752.26	kPa	Joback Method
rinpol	1868.00		NIST Webbook
rinpol	1866.00		NIST Webbook
tb	1090.44	K	Joback Method
tc	1376.76	K	Joback Method
tf	680.74	K	Joback Method
vc	1.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1394.34	J/mol×K	1090.44	Joback Method
cpg	1405.21	J/mol×K	1138.16	Joback Method
cpg	1413.74	J/mol×K	1185.88	Joback Method
cpg	1420.12	J/mol×K	1233.60	Joback Method
cpg	1424.56	J/mol×K	1281.32	Joback Method
cpg	1427.25	J/mol×K	1329.04	Joback Method
cpg	1428.39	J/mol×K	1376.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R394762&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

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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