

Mandelonitrile, rhamnoglucoside (isomer # 1), TFA

Inchi:	InChI=1S/C33H18F21NO18/c34-27(35,36)20(56)66-11-10(65-18(64-9(6-55)8-4-2-1-3-5-
InchiKey:	JFWICXYVYOLOOE-FYASSNCYSA-N
Formula:	C33H18F21NO18
SMILES:	N#CC(OC1OC(COC2OC(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C2OC
Mol. weight [g/mol]:	1115.46

Physical Properties

Property code	Value	Unit	Source
gf	-5633.46	kJ/mol	Joback Method
hf	-6804.00	kJ/mol	Joback Method
hfus	116.11	kJ/mol	Joback Method
hvap	151.51	kJ/mol	Joback Method
log10ws	-8.48		Crippen Method
logp	4.642		Crippen Method
mcvol	544.460	ml/mol	McGowan Method
pc	500.93	kPa	Joback Method
rinpol	2251.00		NIST Webbook
rinpol	2251.00		NIST Webbook
tb	1679.33	K	Joback Method
tc	2944.67	K	Joback Method
tf	1150.97	K	Joback Method
vc	2.200	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1666.92	J/molxK	1679.33	Joback Method
cpg	1450.40	J/molxK	1890.22	Joback Method
cpg	1187.87	J/molxK	2101.11	Joback Method
cpg	892.87	J/molxK	2312.00	Joback Method
cpg	578.97	J/molxK	2522.89	Joback Method
cpg	259.72	J/molxK	2733.78	Joback Method
cpg	-51.34	J/molxK	2944.67	Joback Method

Sources

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=R223893&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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