«alpha»-Terpineol, 6-O-(«alpha»-arabinofuranosyl)-«beta»-D-glucopy TFA

InChI: InChI=1S/C34H27F21O18/c1-8-4-5-9(6-10(8)64-17-14(68-23(59)31(44,45)46)12(66-21(5

InchiKey: QFCQZRLAHCHDOF-BTFPHHTRSA-N

Formula: C34H27F21O18

SMILES: CC1=CCC(C(C)(C)OC2OC(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C2O

Mol. weight [g/mol]: 1122.53

Physical Properties

Property code	Value	Unit	Source
gf	-5808.47	kJ/mol	Joback Method
hf	-7122.73	kJ/mol	Joback Method
hfus	114.03	kJ/mol	Joback Method
hvap	141.28	kJ/mol	Joback Method
log10ws	-9.09		Crippen Method
logp	5.512		Crippen Method
mcvol	565.770	ml/mol	McGowan Method
pc	460.89	kPa	Joback Method
rinpol	2334.00		NIST Webbook
rinpol	2345.00		NIST Webbook
tb	1590.08	K	Joback Method
tc	2706.70	K	Joback Method
tf	1112.43	K	Joback Method
vc	2.260	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1946.42	J/mol×K	1590.08	Joback Method
cpg	1812.33	J/mol×K	1776.18	Joback Method
cpg	1648.94	J/mol×K	1962.29	Joback Method
cpg	1468.80	J/mol×K	2148.39	Joback Method
cpg	1284.47	J/mol×K	2334.49	Joback Method
cpg	1108.51	J/mol×K	2520.60	Joback Method
cpg	953.48	J/mol×K	2706.70	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=R184664&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