

«alpha»-Terpineol, rutinose, TFA

Inchi:	InChI=1S/C34H32F18O16/c1-10-5-7-12(8-6-10)28(3,4)68-21-19(67-27(58)34(50,51)52)1
InchiKey:	PHHGLMDXBUCCT-KLCWCDKESA-N
Formula:	C34H32F18O16
SMILES:	CC1=CCC(C(C)(C)OC2OC(COC3OC(C)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C3OC(=
Mol. weight [g/mol]:	1038.58

Physical Properties

Property code	Value	Unit	Source
gf	-5005.06	kJ/mol	Joback Method
hf	-6287.01	kJ/mol	Joback Method
hfus	107.32	kJ/mol	Joback Method
hvap	136.04	kJ/mol	Joback Method
log10ws	-9.07		Crippen Method
logp	5.859		Crippen Method
mcvol	553.020	ml/mol	McGowan Method
pc	480.29	kPa	Joback Method
rinpol	2241.00		NIST Webbook
rinpol	2251.00		NIST Webbook
tb	1523.48	K	Joback Method
tc	2343.17	K	Joback Method
tf	1032.56	K	Joback Method
vc	2.186	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1957.84	J/mol×K	1523.48	Joback Method
cpg	1865.28	J/mol×K	1660.10	Joback Method
cpg	1747.67	J/mol×K	1796.71	Joback Method
cpg	1609.13	J/mol×K	1933.33	Joback Method
cpg	1453.80	J/mol×K	2069.94	Joback Method
cpg	1285.81	J/mol×K	2206.56	Joback Method
cpg	1109.28	J/mol×K	2343.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R184679&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
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
rlnol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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