Methyl salicylate, Rut, TFA

Inchi: InChI=1S/C32H22F18O18/c1-8-12(63-21(52)27(33,34)35)14(65-23(54)29(39,40)41)16(6
InchiKey: GRVDKAYNFVDHBS-UNENLGJYSA-N
Formula: C32H22F18O18
SMILES: COC(=O)c1ccccc1OC1OC(COC2OC(C)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C2OC(=
Mol. weight [g/mol]: 1036.48

Physical Properties

Property code	Value	Unit	Source
gf	-5200.66	kJ/mol	Joback Method
hf	-6357.35	kJ/mol	Joback Method
hfus	113.33	kJ/mol	Joback Method
hvap	143.60	kJ/mol	Joback Method
log10ws	-7.77		Crippen Method
logp	4.183		Crippen Method
mcvol	523.680	ml/mol	McGowan Method
pc	552.59	kPa	Joback Method
rinpol	2224.00		NIST Webbook
rinpol	2234.00		NIST Webbook
rinpol	2224.00		NIST Webbook
tb	1565.21	K	Joback Method
tc	2459.66	K	Joback Method
tf	1098.04	K	Joback Method
vc	2.082	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1680.61	J/mol×K	1565.21	Joback Method
cpg	1528.06	J/mol×K	1714.29	Joback Method
cpg	1333.71	J/mol×K	1863.36	Joback Method
cpg	1100.01	J/mol×K	2012.44	Joback Method
cpg	829.37	J/mol×K	2161.51	Joback Method
cpg	524.22	J/mol×K	2310.59	Joback Method
cpg	186.99	J/mol×K	2459.66	Joback Method

Sources

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=R394757&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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