Vanillylmandelic acid, acetyl, DTFMBz

Inchi: InChI=1S/C22H18F6O7/c1-11(29)34-17-5-4-14(8-18(17)32-3)19(35-12(2)30)20(31)33-10
InchiKey: JDFUMWWLMVVXDN-UHFFFAOYSA-N
Formula: C22H18F6O7
SMILES: COc1cc(C(OC(C)=O)C(=O)OCc2cc(C(F)(F)F)cc(C(F)(F)F)c2)ccc1OC(C)=O
Mol. weight [g/mol]: 508.36

Physical Properties

Property code	Value	Unit	Source
gf	-1651.72	kJ/mol	Joback Method
hf	-2136.29	kJ/mol	Joback Method
hfus	48.94	kJ/mol	Joback Method
hvap	93.76	kJ/mol	Joback Method
log10ws	-6.46		Crippen Method
logp	5.006		Crippen Method
mcvol	312.130	ml/mol	McGowan Method
pc	1247.73	kPa	Joback Method
rinpol	2272.00		NIST Webbook
rinpol	2272.00		NIST Webbook
tb	1016.05	K	Joback Method
tc	1244.05	K	Joback Method
tf	672.71	K	Joback Method
vc	1.222	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	996.15	J/mol×K	1016.05	Joback Method
cpg	1004.78	J/mol×K	1054.05	Joback Method
cpg	1011.99	J/mol×K	1092.05	Joback Method
cpg	1017.81	J/mol×K	1130.05	Joback Method
cpg	1022.30	J/mol×K	1168.05	Joback Method
cpg	1025.50	J/mol×K	1206.05	Joback Method
cpg	1027.44	J/mol×K	1244.05	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=R539049&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