Tetrahydrocannabinol, TFA

Inchi: InChI=1S/C23H29F3O3/c1-5-6-7-8-15-12-18(28-21(27)23(24,25)26)20-16-11-14(2)9-10-

InchiKey: SRIMOVWPMJEATH-UHFFFAOYSA-N

Formula: C23H29F3O3

SMILES: CCCCCc1cc(OC(=O)C(F)(F)F)c2c(c1)OC(C)(C)C1CCC(C)=CC21

Mol. weight [g/mol]: 410.47

Physical Properties

Property code	Value	Unit	Source
gf	-570.90	kJ/mol	Joback Method
hf	-1115.32	kJ/mol	Joback Method
hfus	48.47	kJ/mol	Joback Method
hvap	80.64	kJ/mol	Joback Method
log10ws	-7.84		Crippen Method
logp	6.498		Crippen Method
mcvol	303.770	ml/mol	McGowan Method
pc	1208.99	kPa	Joback Method
rinpol	2400.00		NIST Webbook
tb	886.81	K	Joback Method
tc	1099.49	K	Joback Method
tf	577.65	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1010.20	J/mol×K	886.81	Joback Method
cpg	1029.54	J/mol×K	922.26	Joback Method
cpg	1048.45	J/mol×K	957.70	Joback Method
cpg	1067.09	J/mol×K	993.15	Joback Method
cpg	1085.63	J/mol×K	1028.60	Joback Method
cpg	1104.23	J/mol×K	1064.04	Joback Method
cpg	1123.06	J/mol×K	1099.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U119842&Units=SI
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

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