Sambunigrin, TFA

Inchi: InChI=1S/C22H13F12NO10/c23-19(24,25)15(36)40-7-10-11(43-16(37)20(26,27)28)12(44
InchiKey: QACJROAZWAFVTJ-GAURVVSWSA-N
Formula: C22H13F12NO10
SMILES: N#CC(OC1OC(COC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C1OC(=O)C(F
Mol. weight [g/mol]: 679.32

Physical Properties

Property code	Value	Unit	Source
gf	-3082.04	kJ/mol	Joback Method
hf	-3760.06	kJ/mol	Joback Method
hfus	68.50	kJ/mol	Joback Method
hvap	104.68	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	3.521		Crippen Method
mcvol	350.340	ml/mol	McGowan Method
pc	947.33	kPa	Joback Method
rinpol	1883.00		NIST Webbook
rinpol	1890.00		NIST Webbook
tb	1164.80	K	Joback Method
tc	1453.63	K	Joback Method
tf	758.73	K	Joback Method
vc	1.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1205.52	J/mol×K	1164.80	Joback Method
cpg	1205.90	J/mol×K	1212.94	Joback Method
cpg	1203.79	J/mol×K	1261.08	Joback Method
cpg	1199.30	J/mol×K	1309.21	Joback Method
cpg	1192.57	J/mol×K	1357.35	Joback Method
cpg	1183.74	J/mol×K	1405.49	Joback Method
cpg	1172.95	J/mol×K	1453.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R223922&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