3,4-Di hydroxyphenylacetic acid, TFA-ME

Inchi: InChI=1S/C13H8F6O6/c1-23-9(20)5-6-2-3-7(24-10(21)12(14,15)16)8(4-6)25-11(22)13(17
InchiKey: PUWAMYRSSMUUBH-UHFFFAOYSA-N
Formula: C13H8F6O6
SMILES: COC(=O)Cc1ccc(OC(=O)C(F)(F)F)c(OC(=O)C(F)(F)F)c1
Mol. weight [g/mol]: 374.19

Physical Properties

Property code	Value	Unit	Source
gf	-1713.21	kJ/mol	Joback Method
hf	-2026.62	kJ/mol	Joback Method
hfus	34.70	kJ/mol	Joback Method
hvap	68.11	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	2.337		Crippen Method
mcvol	203.210	ml/mol	McGowan Method
pc	1959.60	kPa	Joback Method
rinpol	1390.00		NIST Webbook
rinpol	1390.00		NIST Webbook
tb	751.51	K	Joback Method
tc	941.89	K	Joback Method
tf	512.59	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.74	J/mol×K	751.51	Joback Method
cpg	587.36	J/mol×K	783.24	Joback Method
cpg	596.21	J/mol×K	814.97	Joback Method
cpg	604.29	J/mol×K	846.70	Joback Method
cpg	611.64	J/mol×K	878.43	Joback Method
cpg	618.27	J/mol×K	910.16	Joback Method
cpg	624.20	J/mol×K	941.89	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R387165&Units=SI

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