2,3-Dihydroxytoluene, trifluoroacetate

Inchi: InChI=1S/C11H6F6O4/c1-5-3-2-4-6(20-8(18)10(12,13)14)7(5)21-9(19)11(15,16)17/h2-4H
InchiKey: DHLFFAPMPMJESG-UHFFFAOYSA-N
Formula: C11H6F6O4
SMILES: Cc1cccc(OC(=O)C(F)(F)F)c1OC(=O)C(F)(F)F
Mol. weight [g/mol]: 316.15

Physical Properties

Property code	Value	Unit	Source
hfus	26.74	kJ/mol	Joback Method
ie	9.45	eV	Cheméo Relay (1.0)
logp	2.930		Crippen Method
mcvol	167.590	ml/mol	McGowan Method
rinpol	1065.00		NIST Webbook
rinpol	1065.00		NIST Webbook
tb	465.64	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	441.58	J/mol×K	629.46	Joback Method
cpg	451.74	J/mol×K	660.42	Joback Method
cpg	461.19	J/mol×K	691.37	Joback Method
cpg	469.97	J/mol×K	722.33	Joback Method
cpg	478.09	J/mol×K	753.28	Joback Method
cpg	485.59	J/mol×K	784.24	Joback Method
cpg	492.49	J/mol×K	815.20	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25854506&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature