3,5-Bis(trifluoromethyl)phenylacetic acid

Other names: 3,5-bis(trifluoromethyl)phenylacetic acid
Inchi: InChI=1S/C10H6F6O2/c11-9(12,13)6-1-5(3-8(17)18)2-7(4-6)10(14,15)16/h1-2,4H,3H2,(H
InchiKey: PAWSKKHEEYTXSA-UHFFFAOYSA-N
Formula: C10H6F6O2
SMILES: O=C(O)Cc1cc(C(F)(F)F)cc(C(F)(F)F)c1
Mol. weight [g/mol]: 272.14

Physical Properties

Property code	Value	Unit	Source
hfus	24.26	kJ/mol	Joback Method
hvap	79.62	kJ/mol	Cheméo Relay (1.0)
ie	9.51	eV	Cheméo Relay (1.0)
log10ws	-3.90		Cheméo Relay (1.0)
logp	3.351		Crippen Method
mcvol	146.060	ml/mol	McGowan Method
pc	2619.09	kPa	Joback Method
tb	509.37	K	Cheméo Relay (1.0)
tf	408.31	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.29	J/mol×K	600.05	Joback Method
cpg	391.29	J/mol×K	629.05	Joback Method
cpg	399.65	J/mol×K	658.06	Joback Method
cpg	407.42	J/mol×K	687.06	Joback Method
cpg	414.63	J/mol×K	716.06	Joback Method
cpg	421.32	J/mol×K	745.07	Joback Method
cpg	427.52	J/mol×K	774.07	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C85068333&Units=SI
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
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point