

2,4-Bis(trifluoromethyl)benzoic acid

Other names:	2,4-Bis(trifluoromethyl)benzoic acid
Inchi:	InChI=1S/C9H4F6O2/c10-8(11,12)4-1-2-5(7(16)17)6(3-4)9(13,14)15/h1-3H,(H,16,17)
InchiKey:	JTOIZLCQNWDCN-UHFFFAOYSA-N
Formula:	C9H4F6O2
SMILES:	O=C(O)c1ccc(C(F)(F)F)cc1C(F)(F)F
Mol. weight [g/mol]:	258.12

Physical Properties

Property code	Value	Unit	Source
hfus	21.67	kJ/mol	Joback Method
hvap	79.79	kJ/mol	Cheméo Relay (1.0)
ie	10.17	eV	Cheméo Relay (1.0)
log10ws	-3.76		Cheméo Relay (1.0)
logp	3.422		Crippen Method
mcvol	131.970	ml/mol	McGowan Method
tb	491.98	K	Cheméo Relay (1.0)
tf	390.74	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.63	J/mol×K	577.17	Joback Method
cpg	344.96	J/mol×K	606.37	Joback Method
cpg	352.67	J/mol×K	635.57	Joback Method
cpg	359.80	J/mol×K	664.78	Joback Method
cpg	366.39	J/mol×K	693.98	Joback Method
cpg	372.47	J/mol×K	723.18	Joback Method
cpg	378.09	J/mol×K	752.38	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=C32890872&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
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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