2,6-Bis(trifluoromethyl)benzoic acid

Other names: 2,6-di(Trifluoromethyl)benzoic acid
Benzoic acid, 2,6-bis(trifluoromethyl)-
Inchi: InChI=1S/C9H4F6O2/c10-8(11,12)4-2-1-3-5(9(13,14)15)6(4)7(16)17/h1-3H,(H,16,17)
InchiKey: XZNLSDPNMNWCRE-UHFFFAOYSA-N
Formula: C9H4F6O2
SMILES: O=C(O)c1c(C(F)(F)F)cccc1C(F)(F)F
Mol. weight [g/mol]: 258.12
CAS: 24821-22-5

Physical Properties

Property code	Value	Unit	Source
gf	-1310.87	kJ/mol	Joback Method
hf	-1474.47	kJ/mol	Joback Method
hfus	21.67	kJ/mol	Joback Method
hvap	55.16	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.422		Crippen Method
mcvol	131.970	ml/mol	McGowan Method
pc	2896.73	kPa	Joback Method
tb	577.17	K	Joback Method
tc	752.38	K	Joback Method
tf	361.78	K	Joback Method
vc	0.542	m3/kmol	Joback Method

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
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=C24821225&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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