3,5-BIS(TRIFLUOROMETHYL)BENZYL ALCOHOL

Other names: 3,5-di(Trifluoromethyl)benzyl alcohol
Benzenemethanol, 3,5-bis(trifluoromethyl)-
Inchi: InChI=1S/C9H6F6O/c10-8(11,12)6-1-5(4-16)2-7(3-6)9(13,14)15/h1-3,16H,4H2
InchiKey: BJTWPJOGDWRYDD-UHFFFAOYSA-N
Formula: C9H6F6O
SMILES: OCc1cc(C(F)(F)F)cc(C(F)(F)F)c1
Mol. weight [g/mol]: 244.13

Physical Properties

Property code	Value	Unit	Source
hfus	20.07	kJ/mol	Joback Method
ie	9.39	eV	Cheméo Relay (1.0)
logp	3.217		Crippen Method
mcvol	130.400	ml/mol	McGowan Method
tb	451.76	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.98	J/mol×K	523.30	Joback Method
cpg	332.55	J/mol×K	551.11	Joback Method
cpg	341.48	J/mol×K	578.92	Joback Method
cpg	349.82	J/mol×K	606.72	Joback Method
cpg	357.59	J/mol×K	634.53	Joback Method
cpg	364.84	J/mol×K	662.34	Joback Method
cpg	371.59	J/mol×K	690.15	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
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=C32707894&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tb:	Normal Boiling Point Temperature