3,5-Bis(trifluoromethyl)benzylamine

Inchi: InChI=1S/C9H7F6N/c10-8(11,12)6-1-5(4-16)2-7(3-6)9(13,14)15/h1-3H,4,16H2
InchiKey: DHVHORCFFOSRBP-UHFFFAOYSA-N
Formula: C9H7F6N
SMILES: NCc1cc(C(F)(F)F)cc(C(F)(F)F)c1
Mol. weight [g/mol]: 243.15

Physical Properties

Property code	Value	Unit	Source
hfus	21.18	kJ/mol	Joback Method
ie	9.06	eV	Cheméo Relay (1.0)
logp	3.183		Crippen Method
mcvol	134.510	ml/mol	McGowan Method
tb	455.92	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.94	J/mol×K	503.65	Joback Method
cpg	339.47	J/mol×K	534.44	Joback Method
cpg	350.19	J/mol×K	565.22	Joback Method
cpg	360.14	J/mol×K	596.01	Joback Method
cpg	369.36	J/mol×K	626.79	Joback Method
cpg	377.90	J/mol×K	657.58	Joback Method
cpg	385.80	J/mol×K	688.37	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=C42365628&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
tb:	Normal Boiling Point Temperature