3-(Trifluoromethoxy)benzylamine

Inchi: InChI=1S/C8H8F3NO/c9-8(10,11)13-7-3-1-2-6(4-7)5-12/h1-4H,5,12H2
InchiKey: TUPUHSXMDIWJQT-UHFFFAOYSA-N
Formula: C8H8F3NO
SMILES: NCc1cccc(OC(F)(F)F)c1
Mol. weight [g/mol]: 191.15
CAS: 93071-75-1

Physical Properties

Property code	Value	Unit	Source
gf	-500.88	kJ/mol	Joback Method
hf	-678.90	kJ/mol	Joback Method
hfus	18.34	kJ/mol	Joback Method
hvap	45.64	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	2.044		Crippen Method
mcvol	120.980	ml/mol	McGowan Method
pc	3280.28	kPa	Joback Method
tb	503.63	K	Joback Method
tc	705.66	K	Joback Method
tf	328.54	K	Joback Method
vc	0.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.68	J/mol×K	503.63	Joback Method
cpg	291.12	J/mol×K	537.30	Joback Method
cpg	301.85	J/mol×K	570.97	Joback Method
cpg	311.87	J/mol×K	604.64	Joback Method
cpg	321.23	J/mol×K	638.32	Joback Method
cpg	329.95	J/mol×K	671.99	Joback Method
cpg	338.06	J/mol×K	705.66	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=C93071751&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