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
CAS: 32707-89-4

Physical Properties

Property code	Value	Unit	Source
gf	-1181.95	kJ/mol	Joback Method
hf	-1361.89	kJ/mol	Joback Method
hfus	20.07	kJ/mol	Joback Method
hvap	48.41	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.217		Crippen Method
mcvol	130.400	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
tb	523.30	K	Joback Method
tc	690.15	K	Joback Method
tf	311.85	K	Joback Method
vc	0.536	m3/kmol	Joback Method

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

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=C32707894&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