Benzenemethanol, «alpha»-methyl-2-(trifluoromethyl)-

Other names: Benzyl alcohol, «alpha»-methyl-o-(trifluoromethyl)-
«alpha»-Methyl-2-(trifluoromethyl)benzyl alcohol
«alpha»-Methyl-o-trifluoromethylbenzyl alcohol
1-[2-(Trifluoromethyl)phenyl]ethanol

Inchi: InChI=1S/C9H9F3O/c1-6(13)7-4-2-3-5-8(7)9(10,11)12/h2-6,13H,1H3

InchiKey: VGHBIJJTMFYTPY-UHFFFAOYSA-N

Formula: C9H9F3O

SMILES: CC(O)c1ccccc1C(F)(F)F

Mol. weight [g/mol]: 190.16

CAS: 79756-81-3

Physical Properties

Property code	Value	Unit	Source
gf	-593.17	kJ/mol	Joback Method
hf	-758.62	kJ/mol	Joback Method
hfus	15.11	kJ/mol	Joback Method
hvap	51.11	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	2.759		Crippen Method
mcvol	125.090	ml/mol	McGowan Method
pc	3149.09	kPa	Joback Method
tb	523.30	K	Joback Method
tc	706.82	K	Joback Method
tf	280.14	K	Joback Method
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.15	J/mol×K	523.30	Joback Method
cpg	305.96	J/mol×K	553.89	Joback Method
cpg	316.10	J/mol×K	584.47	Joback Method
cpg	325.59	J/mol×K	615.06	Joback Method
cpg	334.47	J/mol×K	645.65	Joback Method

cpg	342.78	J/mol×K	676.24	Joback Method
cpg	350.54	J/mol×K	706.82	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	387.50 ± 0.50	K	0.30	NIST Webbook

Sources

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=C79756813&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume