M-(TRIFLUOROMETHYL)BENZYL ALCOHOL

Other names: 3-Trifluoromethylbenzyl alcohol
Benzenemethanol, 3-(trifluoromethyl)-
3-(trifluoromethyl)benzylic alcohol
Inchi: InChI=1S/C8H7F3O/c9-8(10,11)7-3-1-2-6(4-7)5-12/h1-4,12H,5H2
InchiKey: BXEHKCUWIODEDE-UHFFFAOYSA-N
Formula: C8H7F3O
SMILES: OCc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 176.14

Physical Properties

Property code	Value	Unit	Source
hf	-767.44	kJ/mol	Cheméo Relay (1.0)
hfus	16.04	kJ/mol	Joback Method
hvap	66.63	kJ/mol	Cheméo Relay (1.0)
ie	9.44	eV	Cheméo Relay (1.0)
log10ws	-1.26		Cheméo Relay (1.0)
logp	2.198		Crippen Method
mcvol	111.000	ml/mol	McGowan Method
pc	3484.76	kPa	Joback Method
tb	452.64	K	Cheméo Relay (1.0)
tc	680.71	K	Cheméo Relay (1.0)
tf	291.39	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.83	J/mol×K	500.86	Joback Method
cpg	261.52	J/mol×K	531.14	Joback Method
cpg	270.59	J/mol×K	561.42	Joback Method
cpg	279.08	J/mol×K	591.71	Joback Method
cpg	287.01	J/mol×K	621.99	Joback Method
cpg	294.42	J/mol×K	652.27	Joback Method
cpg	301.34	J/mol×K	682.55	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	341.20	K	0.30	NIST Webbook
tbrp	358.50 ± 1.50	K	0.40	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C349757&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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