

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
CAS:	349-75-7

Physical Properties

Property code	Value	Unit	Source
gf	-599.15	kJ/mol	Joback Method
hf	-732.70	kJ/mol	Joback Method
hfus	16.04	kJ/mol	Joback Method
hvap	49.27	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.198		Crippen Method
mcvol	111.000	ml/mol	McGowan Method
pc	3484.76	kPa	Joback Method
tb	500.86	K	Joback Method
tc	682.55	K	Joback Method
tf	283.87	K	Joback Method
vc	0.438	m3/kmol	Joback Method

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

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=C349757&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

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