

Benzeneethanol, 3-(trifluoromethyl)-

Other names:	Phenethyl alcohol, m-(trifluoromethyl)- 3-(Trifluoromethyl)phenethyl alcohol 2-[m-(Trifluoromethyl)phenyl]ethanol 2-[3-(Trifluoromethyl)phenyl]ethanol m-(Trifluoromethyl)phenethyl alcohol 3-(trifluoromethyl)phenethyl alcohol
Inchi:	InChI=1S/C9H9F3O/c10-9(11,12)8-3-1-2-7(6-8)4-5-13/h1-3,6,13H,4-5H2
InchiKey:	YDKIPCKZKQMDT-UHFFFAOYSA-N
Formula:	C9H9F3O
SMILES:	OCCc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]:	190.16
CAS:	455-01-6

Physical Properties

Property code	Value	Unit	Source
gf	-590.73	kJ/mol	Joback Method
hf	-753.34	kJ/mol	Joback Method
hfus	18.63	kJ/mol	Joback Method
hvap	51.50	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.240		Crippen Method
mcvol	125.090	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
rinpol	1151.00		NIST Webbook
rinpol	1151.00		NIST Webbook
tb	523.74	K	Joback Method
tc	703.63	K	Joback Method
tf	295.14	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.84	J/molxK	523.74	Joback Method

cpg	305.38	J/mol×K	553.72	Joback Method
cpg	315.27	J/mol×K	583.70	Joback Method
cpg	324.54	J/mol×K	613.69	Joback Method
cpg	333.24	J/mol×K	643.67	Joback Method
cpg	341.39	J/mol×K	673.65	Joback Method
cpg	349.03	J/mol×K	703.63	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	375.20	K	1.60	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C455016&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinpola:	Non-polar retention indices
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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