

Trifluoroacetic acid, benzyl ester

Other names:	Acetic acid, trifluoro-, benzyl ester Benzyl trifluoroacetate Trifluoroacetic acid, benzyl ester Benzenemethanol, trifluoroacetate
Inchi:	InChI=1S/C9H7F3O2/c10-9(11,12)8(13)14-6-7-4-2-1-3-5-7/h1-5H,6H2
InchiKey:	HDYQLGLEPPGPEV-UHFFFAOYSA-N
Formula:	C9H7F3O2
SMILES:	O=C(OCc1ccccc1)C(F)(F)F
Mol. weight [g/mol]:	204.15

Physical Properties

Property code	Value	Unit	Source
hf	-861.98	kJ/mol	Cheméo Relay (1.0)
hfus	17.72	kJ/mol	Joback Method
hvap	53.94	kJ/mol	Cheméo Relay (1.0)
ie	9.56	eV	Cheméo Relay (1.0)
log10ws	-1.75		Cheméo Relay (1.0)
logp	2.292		Crippen Method
mcvol	126.660	ml/mol	McGowan Method
pc	3015.64	kPa	Joback Method
rinpol	988.00		NIST Webbook
rinpol	988.00		NIST Webbook
tb	445.54	K	Cheméo Relay (1.0)
tf	231.49	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.68	J/mol×K	502.87	Joback Method
cpg	296.41	J/mol×K	535.70	Joback Method
cpg	307.38	J/mol×K	568.54	Joback Method
cpg	317.62	J/mol×K	601.37	Joback Method
cpg	327.16	J/mol×K	634.20	Joback Method
cpg	336.03	J/mol×K	667.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C351702&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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