2-(Trifluoromethyl)benzyl alcohol

Other names:	o-Trifluoromethylbenzyl alcohol
	Benzenemethanol, 2-(trifluoromethyl)-
	2-(trifluoromethyl)benzylic alcohol
Inchi:	InChI=1S/C8H7F3O/c9-8(10,11)7-4-2-1-3-6(7)5-12/h1-4,12H,5H2
InchiKey:	TWQNSHZTQSLJEE-UHFFFAOYSA-N
Formula:	C8H7F3O
SMILES:	OCc1ccccc1C(F)(F)F
Mol. weight [g/mol]:	176.14
CAS:	346-06-5

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	354.50 ± 1.50	K	0.40	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C346065&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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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