2-Trifluoromethylbenzyl bromide

Other names:	o-Trifluoromethylbenzyl bromide
	Benzene, 1-(bromomethyl)-2-(trifluoromethyl)-
	1-(bromomethyl)-2-(trifluoromethyl)benzene
Inchi:	InChI=1S/C8H6BrF3/c9-5-6-3-1-2-4-7(6)8(10,11)12/h1-4H,5H2
InchiKey:	TXVVVEUSVBLDED-UHFFFAOYSA-N
Formula:	C8H6BrF3
SMILES:	FC(F)(F)c1ccccc1CBr
Mol. weight [g/mol]:	239.03
CAS:	395-44-8

Physical Properties

Property code	Value	Unit	Source
gf	-448.01	kJ/mol	Joback Method
hf	-554.14	kJ/mol	Joback Method
hfus	17.24	kJ/mol	Joback Method
hvap	39.03	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.600		Crippen Method
mcvol	122.630	ml/mol	McGowan Method
pc	3392.03	kPa	Joback Method
tb	474.84	K	Joback Method
tc	683.15	K	Joback Method
tf	282.85	K	Joback Method
vc	0.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.25	J/mol×K	474.84	Joback Method
cpg	252.29	J/mol×K	509.56	Joback Method
cpg	262.49	J/mol×K	544.28	Joback Method
cpg	271.89	J/mol×K	578.99	Joback Method
cpg	280.55	J/mol×K	613.71	Joback Method
cpg	288.52	J/mol×K	648.43	Joback Method

cpg	295.85	J/mol×K	683.15	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	344.00 ± 1.00	K	0.90	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=C395448&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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