3-Trifluoromethylbenzyl bromide

Other names:	m-Trifluoromethylbenzyl bromide
	Benzene, 1-(bromomethyl)-3-(trifluoromethyl)-
	1-(bromomethyl)-3-(trifluoromethyl)benzene
Inchi:	InChI=1S/C8H6BrF3/c9-5-6-2-1-3-7(4-6)8(10,11)12/h1-4H,5H2
InchiKey:	MYYYZNVAUZVXBO-UHFFFAOYSA-N
Formula:	C8H6BrF3
SMILES:	FC(F)(F)c1cccc(CBr)c1
Mol. weight [g/mol]:	239.03
CAS:	402-23-3

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	342.00	K	0.50	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C402233&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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