6-Bromo-«alpha»,«alpha»,«alpha»-trifluoro-m-tolu

Other names:	3-Amino-4-bromobenzotrifluoride
	Benzenamine, 2-bromo-5-(trifluoromethyl)-
	6-Bromo-alpha,alpha,alpha-trifluoro-m-toluidine
	2-Amino-4-trifluoromethyl-1-bromobenzene
Inchi:	InChI=1S/C7H5BrF3N/c8-5-2-1-4(3-6(5)12)7(9,10)11/h1-3H,12H2
InchiKey:	PZDVFXUBTKPFSG-UHFFFAOYSA-N
Formula:	C7H5BrF3N
SMILES:	Nc1cc(C(F)(F)F)ccc1Br
Mol. weight [g/mol]:	240.02
CAS:	454-79-5

Physical Properties

Property code	Value	Unit	Source
gf	-399.61	kJ/mol	Joback Method
hf	-511.18	kJ/mol	Joback Method
hfus	19.46	kJ/mol	Joback Method
hvap	48.11	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.050		Crippen Method
mcvol	118.520	ml/mol	McGowan Method
pc	4010.84	kPa	Joback Method
rinpol	1209.30		NIST Webbook
rinpol	1209.30		NIST Webbook
tb	529.47	K	Joback Method
tc	753.19	K	Joback Method
tf	367.36	K	Joback Method
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.96	J/mol×K	529.47	Joback Method
cpg	258.25	J/mol×K	566.76	Joback Method
cpg	266.76	J/mol×K	604.04	Joback Method

cpg	274.55	J/mol×K	641.33	Joback Method
cpg	281.67	J/mol×K	678.62	Joback Method
cpg	288.17	J/mol×K	715.91	Joback Method
cpg	294.12	J/mol×K	753.19	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	354.50 ± 0.50	K	0.70	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=C454795&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
rinpol:	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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