Benzene, (bromomethyl)pentafluoro-

Other names:	Toluene, «alpha»-bromo-2,3,4,5,6-pentafluoro-
	«alpha»-Bromo-2,3,4,5,6-pentafluorotoluene
	(Bromomethyl)pentafluorobenzene
	Pentafluorobenzyl bromide
	1-Bromomethylpentafluorobenzene
	2,3,4,5,6-Pentafluorobenzyl bromide
	alpha-bromo-2,3,4,5,6-pentafluorotoluene
Inchi:	InChI=1S/C7H2BrF5/c8-1-2-3(9)5(11)7(13)6(12)4(2)10/h1H2
InchiKey:	XDEPVFFKOVDUNO-UHFFFAOYSA-N
Formula:	C7H2BrF5
SMILES:	Fc1c(F)c(F)c(CBr)c(F)c1F
Mol. weight [g/mol]:	260.99
CAS:	1765-40-8

Physical Properties

Property code	Value	Unit	Source
gf	-887.41	kJ/mol	Joback Method
hf	-962.85	kJ/mol	Joback Method
hfus	26.67	kJ/mol	Joback Method
hvap	39.11	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	3.277		Crippen Method
mcvol	112.080	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
rinpol	991.00		NIST Webbook
tb	447.50 ± 0.50	K	NIST Webbook
tb	447.70	K	NIST Webbook
tc	656.64	K	Joback Method
tf	320.42	K	Joback Method
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	214.73	J/mol×K	473.65	Joback Method
cpg	221.23	J/mol×K	504.15	Joback Method
cpg	227.44	J/mol×K	534.65	Joback Method
cpg	233.37	J/mol×K	565.14	Joback Method
cpg	239.03	J/mol×K	595.64	Joback Method
cpg	244.43	J/mol×K	626.14	Joback Method
cpg	249.56	J/mol×K	656.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1765408&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume