

1-Butene, 4-bromo-3-chloro-3,4,4-trifluoro-

Other names:	4-Bromo-3-chloro-3,4,4-trifluorobutene-1
Inchi:	InChI=1S/C4H3BrClF3/c1-2-3(6,7)4(5,8)9/h2H,1H2
InchiKey:	VULPFOSLGWWARI-UHFFFAOYSA-N
Formula:	C4H3BrClF3
SMILES:	C=CC(F)(Cl)C(F)(F)Br
Mol. weight [g/mol]:	223.42
CAS:	374-25-4

Physical Properties

Property code	Value	Unit	Source
gf	-505.72	kJ/mol	Joback Method
hf	-595.70	kJ/mol	Joback Method
hfus	8.73	kJ/mol	Joback Method
hvap	29.61	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	3.065		Crippen Method
mcvol	97.970	ml/mol	McGowan Method
pc	3786.98	kPa	Joback Method
tb	370.00 ± 1.00	K	NIST Webbook
tc	574.02	K	Joback Method
tf	229.41	K	Joback Method
vc	0.384	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	164.63	J/mol×K	382.54	Joback Method
cpg	172.92	J/mol×K	414.45	Joback Method
cpg	180.42	J/mol×K	446.37	Joback Method
cpg	187.21	J/mol×K	478.28	Joback Method
cpg	193.31	J/mol×K	510.20	Joback Method
cpg	198.79	J/mol×K	542.11	Joback Method
cpg	203.70	J/mol×K	574.02	Joback Method

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=C374254&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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