4-Bromo-1,1,2-trifluorobutene-1

Other names: 1-Butene, 4-bromo-1,1,2-trifluoro-
4-Bromo-1,1,2-trifluoro-1-butene
4-bromo-1,1,2-trifluorobut-1-ene
Inchi: InChI=1S/C4H4BrF3/c5-2-1-3(6)4(7)8/h1-2H2
InchiKey: GQCQMFYIFUDARF-UHFFFAOYSA-N
Formula: C4H4BrF3
SMILES: FC(F)=C(F)CCBr
Mol. weight [g/mol]: 188.97
CAS: 10493-44-4

Physical Properties

Property code	Value	Unit	Source
gf	-524.19	kJ/mol	Joback Method
hf	-590.25	kJ/mol	Joback Method
hfus	18.22	kJ/mol	Joback Method
hvap	28.60	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.849		Crippen Method
mcvol	85.730	ml/mol	McGowan Method
pc	3877.12	kPa	Joback Method
tb	372.00 ± 1.00	K	NIST Webbook
tc	530.47	K	Joback Method
tf	163.41	K	Joback Method
vc	0.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	137.91	J/mol×K	358.81	Joback Method
cpg	144.61	J/mol×K	387.42	Joback Method
cpg	150.92	J/mol×K	416.03	Joback Method
cpg	156.86	J/mol×K	444.64	Joback Method
cpg	162.43	J/mol×K	473.25	Joback Method
cpg	167.67	J/mol×K	501.86	Joback Method

cpg	172.59	J/mol×K	530.47	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10493444&Units=SI

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