Butane, 2-bromo-3-fluoro-, (r*,s*)-

Inchi: InChI=1S/C4H8BrF/c1-3(5)4(2)6/h3-4H,1-2H3/t3-,4+/m0/s1
InchiKey: MVQSVOOVCVGPJU-IUYQGCFVSA-N
Formula: C4H8BrF
SMILES: CC(F)C(C)Br
Mol. weight [g/mol]: 155.01
CAS: 57302-16-6

Physical Properties

Property code	Value	Unit	Source
gf	-202.57	kJ/mol	Joback Method
hf	-306.23	kJ/mol	Joback Method
hfus	7.43	kJ/mol	Joback Method
hvap	29.34	kJ/mol	Joback Method
ie	10.21	eV	NIST Webbook
log10ws	-2.01		Crippen Method
logp	2.128		Crippen Method
mcvol	86.490	ml/mol	McGowan Method
pc	4098.62	kPa	Joback Method
tb	355.47	K	Joback Method
tc	539.31	K	Joback Method
tf	165.23	K	Joback Method
vc	0.328	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	135.56	J/mol×K	355.47	Joback Method
cpg	143.62	J/mol×K	386.11	Joback Method
cpg	151.31	J/mol×K	416.75	Joback Method
cpg	158.62	J/mol×K	447.39	Joback Method
cpg	165.59	J/mol×K	478.03	Joback Method
cpg	172.22	J/mol×K	508.67	Joback Method
cpg	178.52	J/mol×K	539.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57302166&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
ie:	Ionization energy
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