2-Fluoro-3-methylbenzyl bromide

Inchi: InChI=1S/C8H8BrF/c1-6-3-2-4-7(5-9)8(6)10/h2-4H,5H2,1H3
InchiKey: DCGWFNZSJBIAKE-UHFFFAOYSA-N
Formula: C8H8BrF
SMILES: Cc1cccc(CBr)c1F
Mol. weight [g/mol]: 203.05
CAS: 151412-12-3

Physical Properties

Property code	Value	Unit	Source
gf	-70.86	kJ/mol	Joback Method
hf	-164.64	kJ/mol	Joback Method
hfus	18.10	kJ/mol	Joback Method
hvap	42.62	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.029		Crippen Method
mcvol	119.090	ml/mol	McGowan Method
pc	3624.61	kPa	Joback Method
tb	484.51	K	Joback Method
tc	703.28	K	Joback Method
tf	291.77	K	Joback Method
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.28	J/mol×K	484.51	Joback Method
cpg	231.96	J/mol×K	520.97	Joback Method
cpg	241.99	J/mol×K	557.43	Joback Method
cpg	251.42	J/mol×K	593.90	Joback Method
cpg	260.26	J/mol×K	630.36	Joback Method
cpg	268.55	J/mol×K	666.82	Joback Method
cpg	276.31	J/mol×K	703.28	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=C151412123&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