3-(Trifluoromethoxy)benzyl bromide

Inchi: InChI=1S/C8H6BrF3O/c9-5-6-2-1-3-7(4-6)13-8(10,11)12/h1-4H,5H2
InchiKey: QSIVWRRHVXSDNE-UHFFFAOYSA-N
Formula: C8H6BrF3O
SMILES: FC(F)(F)Oc1cccc(CBr)c1
Mol. weight [g/mol]: 255.03
CAS: 159689-88-0

Physical Properties

Property code	Value	Unit	Source
gf	-553.01	kJ/mol	Joback Method
hf	-686.36	kJ/mol	Joback Method
hfus	18.43	kJ/mol	Joback Method
hvap	41.44	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.480		Crippen Method
mcvol	128.500	ml/mol	McGowan Method
pc	3325.84	kPa	Joback Method
tb	497.26	K	Joback Method
tc	703.82	K	Joback Method
tf	305.08	K	Joback Method
vc	0.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.26	J/mol×K	497.26	Joback Method
cpg	273.92	J/mol×K	531.69	Joback Method
cpg	283.84	J/mol×K	566.11	Joback Method
cpg	293.06	J/mol×K	600.54	Joback Method
cpg	301.60	J/mol×K	634.97	Joback Method
cpg	309.52	J/mol×K	669.39	Joback Method
cpg	316.84	J/mol×K	703.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C159689880&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume