4-Bromobenzyl 2,2,2-trifluoroacetate

Other names: 4-Bromobenzyl alcohol, trifluoroacetate
Inchi: InChI=1S/C9H6BrF3O2/c10-7-3-1-6(2-4-7)5-15-8(14)9(11,12)13/h1-4H,5H2
InchiKey: ANOPWAXGWOMPNH-UHFFFAOYSA-N
Formula: C9H6BrF3O2
SMILES: O=C(OCc1ccc(Br)cc1)C(F)(F)F
Mol. weight [g/mol]: 283.04
CAS: 344884-23-7

Physical Properties

Property code	Value	Unit	Source
gf	-673.51	kJ/mol	Joback Method
hf	-819.58	kJ/mol	Joback Method
hfus	22.62	kJ/mol	Joback Method
hvap	50.41	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.055		Crippen Method
mcvol	144.160	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
rinpol	1272.00		NIST Webbook
rinpol	1272.00		NIST Webbook
tb	574.01	K	Joback Method
tc	785.98	K	Joback Method
tf	366.28	K	Joback Method
vc	0.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	319.70	J/mol×K	574.01	Joback Method
cpg	329.97	J/mol×K	609.34	Joback Method
cpg	339.47	J/mol×K	644.67	Joback Method
cpg	348.23	J/mol×K	679.99	Joback Method
cpg	356.31	J/mol×K	715.32	Joback Method
cpg	363.75	J/mol×K	750.65	Joback Method

cpg	370.57	J/mol×K	785.98	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=C344884237&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume