N-benzyl-1,1,1-trifluoromethanesulphonamide

Inchi: InChI=1S/C8H8F3NO2S/c9-8(10,11)15(13,14)12-6-7-4-2-1-3-5-7/h1-5,12H,6H2
InchiKey: IJHVVEQTOXFGCL-UHFFFAOYSA-N
Formula: C8H8F3NO2S
SMILES: O=S(=O)(NCc1ccccc1)C(F)(F)F
Mol. weight [g/mol]: 239.22
CAS: 36457-58-6

Physical Properties

Property code	Value	Unit	Source
gf	-831.85	kJ/mol	Joback Method
hf	-968.88	kJ/mol	Joback Method
hfus	28.82	kJ/mol	Joback Method
hvap	57.00	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	1.626		Crippen Method
mcvol	143.200	ml/mol	McGowan Method
pc	3891.64	kPa	Joback Method
tb	501.65	K	Joback Method
tc	689.25	K	Joback Method
tf	301.75	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.71	J/mol×K	501.65	Joback Method
cpg	335.34	J/mol×K	532.92	Joback Method
cpg	347.15	J/mol×K	564.18	Joback Method
cpg	358.18	J/mol×K	595.45	Joback Method
cpg	368.46	J/mol×K	626.71	Joback Method
cpg	378.01	J/mol×K	657.98	Joback Method
cpg	386.85	J/mol×K	689.25	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=C36457586&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