Trifluoroacetamide, N-[1-(2-methoxyphenyl)ethyl]

Inchi: InChI=1S/C9H8F3NO2/c1-15-7-5-3-2-4-6(7)13-8(14)9(10,11)12/h2-5H,1H3,(H,13,14)
InchiKey: MYPKUDNIQPOXHU-UHFFFAOYSA-N
Formula: C9H8F3NO2
SMILES: COc1ccccc1NC(=O)C(F)(F)F
Mol. weight [g/mol]: 219.16

Physical Properties

Property code	Value	Unit	Source
gf	-598.44	kJ/mol	Joback Method
hf	-792.44	kJ/mol	Joback Method
hfus	22.43	kJ/mol	Joback Method
hvap	50.41	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.196		Crippen Method
mcvol	136.640	ml/mol	McGowan Method
pc	3009.03	kPa	Joback Method
rinpol	1386.00		NIST Webbook
rinpol	1386.00		NIST Webbook
tb	558.02	K	Joback Method
tc	757.27	K	Joback Method
tf	359.14	K	Joback Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.61	J/mol×K	558.02	Joback Method
cpg	340.98	J/mol×K	591.23	Joback Method
cpg	351.60	J/mol×K	624.44	Joback Method
cpg	361.52	J/mol×K	657.64	Joback Method
cpg	370.75	J/mol×K	690.85	Joback Method
cpg	379.33	J/mol×K	724.06	Joback Method
cpg	387.29	J/mol×K	757.27	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=R74042&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