1-Methylcyclohexanol, trifluoroacetate

Inchi: InChI=1S/C9H13F3O2/c1-8(5-3-2-4-6-8)14-7(13)9(10,11)12/h2-6H2,1H3
InchiKey: XHWQUVQVTFUQSG-UHFFFAOYSA-N
Formula: C9H13F3O2
SMILES: CC1(OC(=O)C(F)(F)F)CCCCC1
Mol. weight [g/mol]: 210.19

Physical Properties

Property code	Value	Unit	Source
gf	-771.65	kJ/mol	Joback Method
hf	-1001.41	kJ/mol	Joback Method
hfus	9.22	kJ/mol	Joback Method
hvap	40.31	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	2.815		Crippen Method
mcvol	139.560	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
rinpol	928.00		NIST Webbook
tb	495.98	K	Joback Method
tc	693.88	K	Joback Method
tf	298.82	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.06	J/mol×K	495.98	Joback Method
cpg	351.91	J/mol×K	528.96	Joback Method
cpg	366.69	J/mol×K	561.95	Joback Method
cpg	380.49	J/mol×K	594.93	Joback Method
cpg	393.42	J/mol×K	627.91	Joback Method
cpg	405.55	J/mol×K	660.90	Joback Method
cpg	416.98	J/mol×K	693.88	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=U376255&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