1-Methylcyclohexanol, pentafluoropropionate

Inchi: InChI=1S/C10H13F5O2/c1-8(5-3-2-4-6-8)17-7(16)9(11,12)10(13,14)15/h2-6H2,1H3
InchiKey: XADWRGNABJATCD-UHFFFAOYSA-N
Formula: C10H13F5O2
SMILES: CC1(OC(=O)C(F)(F)C(F)(F)F)CCCCC1
Mol. weight [g/mol]: 260.20

Physical Properties

Property code	Value	Unit	Source
gf	-1150.01	kJ/mol	Joback Method
hf	-1423.02	kJ/mol	Joback Method
hfus	10.55	kJ/mol	Joback Method
hvap	39.61	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	3.450		Crippen Method
mcvol	157.190	ml/mol	McGowan Method
pc	2336.03	kPa	Joback Method
rinpol	947.00		NIST Webbook
rinpol	947.00		NIST Webbook
tb	514.17	K	Joback Method
tc	702.02	K	Joback Method
tf	313.69	K	Joback Method
vc	0.619	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.84	J/mol×K	514.17	Joback Method
cpg	417.91	J/mol×K	545.48	Joback Method
cpg	432.85	J/mol×K	576.79	Joback Method
cpg	446.76	J/mol×K	608.09	Joback Method
cpg	459.74	J/mol×K	639.40	Joback Method
cpg	471.89	J/mol×K	670.71	Joback Method
cpg	483.30	J/mol×K	702.02	Joback Method

Sources

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=U376254&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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