1-Methylcyclohexanol, heptafluorobutyrate

Inchi: InChI=1S/C11H13F7O2/c1-8(5-3-2-4-6-8)20-7(19)9(12,13)10(14,15)11(16,17)18/h2-6H2
InchiKey: KQMFUMNYSRKOTO-UHFFFAOYSA-N
Formula: C11H13F7O2
SMILES: CC1(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)CCCCC1
Mol. weight [g/mol]: 310.21

Physical Properties

Property code	Value	Unit	Source
gf	-1528.37	kJ/mol	Joback Method
hf	-1844.63	kJ/mol	Joback Method
hfus	11.89	kJ/mol	Joback Method
hvap	38.91	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.085		Crippen Method
mcvol	174.820	ml/mol	McGowan Method
pc	2000.12	kPa	Joback Method
rinpol	992.00		NIST Webbook
tb	532.36	K	Joback Method
tc	711.36	K	Joback Method
tf	328.56	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.16	J/mol×K	532.36	Joback Method
cpg	485.24	J/mol×K	562.19	Joback Method
cpg	500.17	J/mol×K	592.03	Joback Method
cpg	514.05	J/mol×K	621.86	Joback Method
cpg	526.97	J/mol×K	651.69	Joback Method
cpg	539.05	J/mol×K	681.52	Joback Method
cpg	550.36	J/mol×K	711.36	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=U376253&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