Borneol, pentafluoropropionate

Inchi: InChI=1S/C13H17F5O2/c1-10(2)7-4-5-11(10,3)8(6-7)20-9(19)12(14,15)13(16,17)18/h7-8
InchiKey: YAHWCTNCIHKPIS-UHFFFAOYSA-N
Formula: C13H17F5O2
SMILES: CC1(C)C2CCC1(C)C(OC(=O)C(F)(F)C(F)(F)F)C2
Mol. weight [g/mol]: 300.26

Physical Properties

Property code	Value	Unit	Source
gf	-1060.71	kJ/mol	Joback Method
hf	-1425.26	kJ/mol	Joback Method
hfus	16.50	kJ/mol	Joback Method
hvap	44.09	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	3.942		Crippen Method
mcvol	188.600	ml/mol	McGowan Method
pc	1893.65	kPa	Joback Method
rinpol	1143.00		NIST Webbook
tb	571.91	K	Joback Method
tc	760.07	K	Joback Method
tf	387.90	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	534.59	J/mol×K	571.91	Joback Method
cpg	551.53	J/mol×K	603.27	Joback Method
cpg	567.31	J/mol×K	634.63	Joback Method
cpg	582.10	J/mol×K	665.99	Joback Method
cpg	596.09	J/mol×K	697.35	Joback Method
cpg	609.44	J/mol×K	728.71	Joback Method
cpg	622.35	J/mol×K	760.07	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=U375536&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