Isoborneol,heptafluorobutyrate (ester)

Other names: Borneol, heptafluorobutanoate
Inchi: InChI=1S/C14H17F7O2/c1-10(2)7-4-5-11(10,3)8(6-7)23-9(22)12(15,16)13(17,18)14(19,2
InchiKey: KOALQGAPEWNVJF-UHFFFAOYSA-N
Formula: C14H17F7O2
SMILES: CC1(C)C2CCC1(C)C(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)C2
Mol. weight [g/mol]: 350.27

Physical Properties

Property code	Value	Unit	Source
gf	-1439.07	kJ/mol	Joback Method
hf	-1846.87	kJ/mol	Joback Method
hfus	17.84	kJ/mol	Joback Method
hvap	43.39	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.577		Crippen Method
mcvol	206.230	ml/mol	McGowan Method
pc	1645.76	kPa	Joback Method
rinpol	1198.00		NIST Webbook
rinpol	1198.00		NIST Webbook
tb	590.10	K	Joback Method
tc	770.09	K	Joback Method
tf	402.77	K	Joback Method
vc	0.837	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.92	J/mol×K	590.10	Joback Method
cpg	621.54	J/mol×K	620.10	Joback Method
cpg	637.04	J/mol×K	650.10	Joback Method
cpg	651.58	J/mol×K	680.10	Joback Method
cpg	665.35	J/mol×K	710.10	Joback Method
cpg	678.50	J/mol×K	740.09	Joback Method
cpg	691.21	J/mol×K	770.09	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=U245883&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