Menthol, heptafluorobutanoate

Inchi: InChI=1S/C14H19F7O2/c1-7(2)9-5-4-8(3)6-10(9)23-11(22)12(15,16)13(17,18)14(19,20)2
InchiKey: HXIYDRJIRXBMIU-AEJSXWLSSA-N
Formula: C14H19F7O2
SMILES: CC1CCC(C(C)C)C(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)C1
Mol. weight [g/mol]: 352.29

Physical Properties

Property code	Value	Unit	Source
gf	-1515.48	kJ/mol	Joback Method
hf	-1967.75	kJ/mol	Joback Method
hfus	24.58	kJ/mol	Joback Method
hvap	45.73	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.823		Crippen Method
mcvol	217.090	ml/mol	McGowan Method
pc	1449.04	kPa	Joback Method
rinpol	1200.00		NIST Webbook
tb	590.98	K	Joback Method
tc	762.61	K	Joback Method
tf	314.99	K	Joback Method
vc	0.862	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.94	J/mol×K	590.98	Joback Method
cpg	644.24	J/mol×K	619.58	Joback Method
cpg	661.47	J/mol×K	648.19	Joback Method
cpg	677.66	J/mol×K	676.79	Joback Method
cpg	692.87	J/mol×K	705.40	Joback Method
cpg	707.13	J/mol×K	734.00	Joback Method
cpg	720.48	J/mol×K	762.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R335481&Units=SI
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

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