3-Buten-2-ol, pentafluoropropionate

Inchi: InChI=1S/C7H7F5O2/c1-3-4(2)14-5(13)6(8,9)7(10,11)12/h3-4H,1H2,2H3
InchiKey: LICUIFILUIGFCR-UHFFFAOYSA-N
Formula: C7H7F5O2
SMILES: C=CC(C)OC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 218.12

Physical Properties

Property code	Value	Unit	Source
gf	-1108.83	kJ/mol	Joback Method
hf	-1310.51	kJ/mol	Joback Method
hfus	12.44	kJ/mol	Joback Method
hvap	32.60	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.302		Crippen Method
mcvol	121.480	ml/mol	McGowan Method
pc	2548.19	kPa	Joback Method
rinpol	719.50		NIST Webbook
rinpol	719.50		NIST Webbook
tb	421.98	K	Joback Method
tc	582.58	K	Joback Method
tf	231.84	K	Joback Method
vc	0.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.97	J/mol×K	421.98	Joback Method
cpg	279.54	J/mol×K	448.75	Joback Method
cpg	289.52	J/mol×K	475.51	Joback Method
cpg	298.93	J/mol×K	502.28	Joback Method
cpg	307.79	J/mol×K	529.05	Joback Method
cpg	316.12	J/mol×K	555.81	Joback Method
cpg	323.96	J/mol×K	582.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352687&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

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