3-Buten-1-ol, pentafluoropropionate

Inchi: InChI=1S/C7H7F5O2/c1-2-3-4-14-5(13)6(8,9)7(10,11)12/h2H,1,3-4H2
InchiKey: VLNYKURGUYTUPW-UHFFFAOYSA-N
Formula: C7H7F5O2
SMILES: C=CCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 218.12

Physical Properties

Property code	Value	Unit	Source
gf	-1106.39	kJ/mol	Joback Method
hf	-1305.23	kJ/mol	Joback Method
hfus	15.96	kJ/mol	Joback Method
hvap	32.98	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.303		Crippen Method
mcvol	121.480	ml/mol	McGowan Method
pc	2527.73	kPa	Joback Method
rinpol	738.50		NIST Webbook
rinpol	738.50		NIST Webbook
tb	422.42	K	Joback Method
tc	579.68	K	Joback Method
tf	246.84	K	Joback Method
vc	0.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.94	J/mol×K	422.42	Joback Method
cpg	279.21	J/mol×K	448.63	Joback Method
cpg	288.92	J/mol×K	474.84	Joback Method
cpg	298.09	J/mol×K	501.05	Joback Method
cpg	306.74	J/mol×K	527.26	Joback Method
cpg	314.88	J/mol×K	553.47	Joback Method
cpg	322.55	J/mol×K	579.68	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=U352272&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