3-Methyl-2-buten-1-ol, pentafluoropropionate

Inchi: InChI=1S/C8H9F5O2/c1-5(2)3-4-15-6(14)7(9,10)8(11,12)13/h3H,4H2,1-2H3
InchiKey: IHVNTTPIHTZFEC-UHFFFAOYSA-N
Formula: C8H9F5O2
SMILES: CC(C)=CCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 232.15

Physical Properties

Property code	Value	Unit	Source
gf	-1114.14	kJ/mol	Joback Method
hf	-1343.87	kJ/mol	Joback Method
hfus	18.73	kJ/mol	Joback Method
hvap	35.92	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.693		Crippen Method
mcvol	135.570	ml/mol	McGowan Method
pc	2333.78	kPa	Joback Method
rinpol	936.60		NIST Webbook
tb	452.66	K	Joback Method
tc	616.38	K	Joback Method
tf	240.83	K	Joback Method
vc	0.556	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.99	J/mol×K	452.66	Joback Method
cpg	321.47	J/mol×K	479.95	Joback Method
cpg	332.28	J/mol×K	507.23	Joback Method
cpg	342.46	J/mol×K	534.52	Joback Method
cpg	352.03	J/mol×K	561.81	Joback Method
cpg	361.02	J/mol×K	589.10	Joback Method
cpg	369.47	J/mol×K	616.38	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=U352702&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