1-Propoxypropan-2-ol, pentafluoropropionate

Inchi: InChI=1S/C9H13F5O3/c1-3-4-16-5-6(2)17-7(15)8(10,11)9(12,13)14/h6H,3-5H2,1-2H3
InchiKey: ITZJIAZTWAVNOD-UHFFFAOYSA-N
Formula: C9H13F5O3
SMILES: CCCOCC(C)OC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 264.19

Physical Properties

Property code	Value	Unit	Source
gf	-1284.83	kJ/mol	Joback Method
hf	-1609.44	kJ/mol	Joback Method
hfus	20.09	kJ/mol	Joback Method
hvap	40.13	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.542		Crippen Method
mcvol	159.830	ml/mol	McGowan Method
pc	2007.30	kPa	Joback Method
rinpol	935.00		NIST Webbook
rinpol	935.00		NIST Webbook
tb	493.48	K	Joback Method
tc	650.28	K	Joback Method
tf	278.37	K	Joback Method
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.32	J/mol×K	493.48	Joback Method
cpg	407.68	J/mol×K	519.61	Joback Method
cpg	419.46	J/mol×K	545.75	Joback Method
cpg	430.68	J/mol×K	571.88	Joback Method
cpg	441.35	J/mol×K	598.02	Joback Method
cpg	451.50	J/mol×K	624.15	Joback Method
cpg	461.13	J/mol×K	650.28	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=U378343&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