

1-Ethoxy-2-propanol, heptafluorobutyrate

Inchi:	InChI=1S/C9H11F7O3/c1-3-18-4-5(2)19-6(17)7(10,11)8(12,13)9(14,15)16/h5H,3-4H2,1-2
InchiKey:	GMZTTYLEJJXPBU-UHFFFAOYSA-N
Formula:	C9H11F7O3
SMILES:	CCOCC(C)OC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	300.17

Physical Properties

Property code	Value	Unit	Source
gf	-1671.61	kJ/mol	Joback Method
hf	-2010.41	kJ/mol	Joback Method
hfus	18.84	kJ/mol	Joback Method
hvap	37.20	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.788		Crippen Method
mcvol	163.370	ml/mol	McGowan Method
pc	1885.44	kPa	Joback Method
rinpol	902.00		NIST Webbook
rinpol	902.00		NIST Webbook
tb	488.79	K	Joback Method
tc	640.13	K	Joback Method
tf	281.97	K	Joback Method
vc	0.668	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	414.60	J/mol×K	488.79	Joback Method
cpg	426.81	J/mol×K	514.01	Joback Method
cpg	438.38	J/mol×K	539.24	Joback Method
cpg	449.34	J/mol×K	564.46	Joback Method
cpg	459.71	J/mol×K	589.68	Joback Method
cpg	469.50	J/mol×K	614.90	Joback Method
cpg	478.75	J/mol×K	640.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378338&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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