

2-Ethoxyethyl 2,2,3,3,4,4,4-heptafluorobutanoate

Other names:	2-Ethoxyethanol, heptafluorobutyrate
Inchi:	InChI=1S/C8H9F7O3/c1-2-17-3-4-18-5(16)6(9,10)7(11,12)8(13,14)15/h2-4H2,1H3
InchiKey:	IYICRDHKBXCVD-UHFFFAOYSA-N
Formula:	C8H9F7O3
SMILES:	CCOCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	286.14

Physical Properties

Property code	Value	Unit	Source
gf	-1677.59	kJ/mol	Joback Method
hf	-1984.49	kJ/mol	Joback Method
hfus	19.77	kJ/mol	Joback Method
hvap	35.36	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.399		Crippen Method
mcvol	149.280	ml/mol	McGowan Method
pc	2038.23	kPa	Joback Method
rinpol	844.10		NIST Webbook
rinpol	844.10		NIST Webbook
tb	466.35	K	Joback Method
tc	615.16	K	Joback Method
tf	285.70	K	Joback Method
vc	0.619	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.07	J/mol×K	466.35	Joback Method
cpg	381.34	J/mol×K	491.15	Joback Method
cpg	392.01	J/mol×K	515.95	Joback Method
cpg	402.12	J/mol×K	540.75	Joback Method
cpg	411.68	J/mol×K	565.56	Joback Method
cpg	420.72	J/mol×K	590.36	Joback Method
cpg	429.25	J/mol×K	615.16	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U352015&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
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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