2-Hydroxyethyl 2,2,3,3,4,4,4-heptafluorobutanoate

Other names: Ethylene glycol, mono(heptafluorobutyrate)
2-Hydroxyethyl 2,2,3,3,4,4,4-heptafluoroabutanoate

Inchi: InChI=1S/C6H5F7O3/c7-4(8,3(15)16-2-1-14)5(9,10)6(11,12)13/h14H,1-2H2

InchiKey: YXNNHFIKNIKAAE-UHFFFAOYSA-N

Formula: C6H5F7O3

SMILES: O=C(OCCO)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 258.09

Physical Properties

Property code	Value	Unit	Source
gf	-1726.25	kJ/mol	Joback Method
hf	-1963.22	kJ/mol	Joback Method
hfus	17.49	kJ/mol	Joback Method
hvap	45.18	kJ/mol	Joback Method
log10ws	-1.75		Crippen Method
logp	1.355		Crippen Method
mcvol	121.100	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
rinpol	829.10		NIST Webbook
rinpol	829.10		NIST Webbook
tb	490.35	K	Joback Method
tc	637.41	K	Joback Method
tf	301.75	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.05	J/mol×K	490.35	Joback Method
cpg	322.30	J/mol×K	514.86	Joback Method
cpg	330.03	J/mol×K	539.37	Joback Method
cpg	337.27	J/mol×K	563.88	Joback Method
cpg	344.04	J/mol×K	588.39	Joback Method
cpg	350.36	J/mol×K	612.90	Joback Method

cpg	356.26	J/mol×K	637.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352002&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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