2-(2-Hydroxyethoxy)ethyl 2,2,3,3,4,4,4-heptafluorobutanoate

Other names: Diethylene glycol, mono(heptafluorobutyrate)
Inchi: InChI=1S/C8H9F7O4/c9-6(10,7(11,12)8(13,14)15)5(17)19-4-3-18-2-1-16/h16H,1-4H2
InchiKey: LXOBPHOXJWCRKO-UHFFFAOYSA-N
Formula: C8H9F7O4
SMILES: O=C(OCCOCCO)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 302.14

Physical Properties

Property code	Value	Unit	Source
gf	-1814.41	kJ/mol	Joback Method
hf	-2136.72	kJ/mol	Joback Method
hfus	23.86	kJ/mol	Joback Method
hvap	52.04	kJ/mol	Joback Method
log10ws	-1.68		Crippen Method
logp	1.371		Crippen Method
mcvol	155.150	ml/mol	McGowan Method
pc	2218.71	kPa	Joback Method
rinpol	1059.10		NIST Webbook
rinpol	1059.10		NIST Webbook
tb	558.53	K	Joback Method
tc	706.90	K	Joback Method
tf	346.52	K	Joback Method
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.52	J/mol×K	558.53	Joback Method
cpg	434.90	J/mol×K	583.26	Joback Method
cpg	443.75	J/mol×K	607.99	Joback Method
cpg	452.10	J/mol×K	632.72	Joback Method
cpg	459.97	J/mol×K	657.45	Joback Method
cpg	467.37	J/mol×K	682.18	Joback Method
cpg	474.34	J/mol×K	706.90	Joback Method

Sources

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=U352003&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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