2-Octanol, 3,3,4,4,5,5,6,6,7,7,8,8-dodecafluoro

Inchi: InChI=1S/C8H6F12O/c1-2(21)4(11,12)6(15,16)8(19,20)7(17,18)5(13,14)3(9)10/h2-3,21H
InchiKey: HRWGQHSSZRFTGP-UHFFFAOYSA-N
Formula: C8H6F12O
SMILES: CC(O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)F
Mol. weight [g/mol]: 346.11
CAS: 156122-84-8

Physical Properties

Property code	Value	Unit	Source
gf	-2448.74	kJ/mol	Joback Method
hf	-2768.31	kJ/mol	Joback Method
hfus	13.41	kJ/mol	Joback Method
hvap	33.02	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	3.809		Crippen Method
mcvol	150.690	ml/mol	McGowan Method
pc	1853.11	kPa	Joback Method
tb	448.83	K	Joback Method
tc	576.27	K	Joback Method
tf	229.92	K	Joback Method
vc	0.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.51	J/mol×K	448.83	Joback Method
cpg	412.71	J/mol×K	470.07	Joback Method
cpg	423.21	J/mol×K	491.31	Joback Method
cpg	433.05	J/mol×K	512.55	Joback Method
cpg	442.25	J/mol×K	533.79	Joback Method
cpg	450.84	J/mol×K	555.03	Joback Method
cpg	458.86	J/mol×K	576.27	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=C156122848&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume