2-Octanol, heptafluorobutyrate

Inchi: InChI=1S/C12H17F7O2/c1-3-4-5-6-7-8(2)21-9(20)10(13,14)11(15,16)12(17,18)19/h8H,3-
InchiKey: CQNVNDNWIKZAAI-UHFFFAOYSA-N
Formula: C12H17F7O2
SMILES: CCCCCCC(C)OC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 326.25

Physical Properties

Property code	Value	Unit	Source
gf	-1541.35	kJ/mol	Joback Method
hf	-1940.11	kJ/mol	Joback Method
hfus	25.42	kJ/mol	Joback Method
hvap	41.47	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.721		Crippen Method
mcvol	199.770	ml/mol	McGowan Method
pc	1509.33	kPa	Joback Method
rinpol	1051.70		NIST Webbook
rinpol	1051.70		NIST Webbook
rinpol	1032.00		NIST Webbook
rinpol	1032.00		NIST Webbook
ripol	1101.00		NIST Webbook
ripol	1101.00		NIST Webbook
tb	535.01	K	Joback Method
tc	685.56	K	Joback Method
tf	293.55	K	Joback Method
vc	0.819	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	529.93	J/mol×K	535.01	Joback Method
cpg	544.18	J/mol×K	560.10	Joback Method
cpg	557.68	J/mol×K	585.19	Joback Method
cpg	570.47	J/mol×K	610.28	Joback Method

cpg	582.58	J/mol×K	635.37	Joback Method
cpg	594.03	J/mol×K	660.47	Joback Method
cpg	604.87	J/mol×K	685.56	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=U352370&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume