2-Decanol, pentafluoropropionate

Inchi: InChI=1S/C13H21F5O2/c1-3-4-5-6-7-8-9-10(2)20-11(19)12(14,15)13(16,17)18/h10H,3-9
InchiKey: KXQIIMVUPLXMKM-UHFFFAOYSA-N
Formula: C13H21F5O2
SMILES: CCCCCCCCC(C)OC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 304.30

Physical Properties

Property code	Value	Unit	Source
gf	-1146.15	kJ/mol	Joback Method
hf	-1559.78	kJ/mol	Joback Method
hfus	29.26	kJ/mol	Joback Method
hvap	46.62	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	4.866		Crippen Method
mcvol	210.320	ml/mol	McGowan Method
pc	1480.43	kPa	Joback Method
rinpol	1204.20		NIST Webbook
tb	562.58	K	Joback Method
tc	717.83	K	Joback Method
tf	301.22	K	Joback Method
vc	0.850	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.18	J/mol×K	562.58	Joback Method
cpg	576.26	J/mol×K	588.46	Joback Method
cpg	590.61	J/mol×K	614.33	Joback Method
cpg	604.27	J/mol×K	640.21	Joback Method
cpg	617.26	J/mol×K	666.08	Joback Method
cpg	629.60	J/mol×K	691.96	Joback Method
cpg	641.33	J/mol×K	717.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352327&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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