Pentafluoropropionic acid, decyl ester

Other names: Decyl pentafluoropropionate
Inchi: InChI=1S/C13H21F5O2/c1-2-3-4-5-6-7-8-9-10-20-11(19)12(14,15)13(16,17)18/h2-10H2,
InchiKey: VVIWDHAVGIYAEE-UHFFFAOYSA-N
Formula: C13H21F5O2
SMILES: CCCCCCCCCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 304.30
CAS: 959000-65-8

Physical Properties

Property code	Value	Unit	Source
gf	-1143.71	kJ/mol	Joback Method
hf	-1554.50	kJ/mol	Joback Method
hfus	32.78	kJ/mol	Joback Method
hvap	47.01	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	4.868		Crippen Method
mcvol	210.320	ml/mol	McGowan Method
pc	1471.36	kPa	Joback Method
rinpol	1256.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1262.90		NIST Webbook
ripol	1311.00		NIST Webbook
tb	563.02	K	Joback Method
tc	716.02	K	Joback Method
tf	316.22	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	560.89	J/mol×K	563.02	Joback Method
cpg	575.70	J/mol×K	588.52	Joback Method
cpg	589.81	J/mol×K	614.02	Joback Method
cpg	603.25	J/mol×K	639.52	Joback Method

cpg	616.04	J/mol×K	665.02	Joback Method
cpg	628.21	J/mol×K	690.52	Joback Method
cpg	639.79	J/mol×K	716.02	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=C959000658&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume