Undecyl 2,3,4,5,6-pentafluorobenzoate

Other names: undecyl pentafluorobenzoate
Inchi: InChI=1S/C18H23F5O2/c1-2-3-4-5-6-7-8-9-10-11-25-18(24)12-13(19)15(21)17(23)16(22
InchiKey: PAWOTZAVMHFMJY-UHFFFAOYSA-N
Formula: C18H23F5O2
SMILES: CCCCCCCCCCCOC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 366.37

Physical Properties

Property code	Value	Unit	Source
gf	-1043.03	kJ/mol	Joback Method
hf	-1461.02	kJ/mol	Joback Method
hfus	52.66	kJ/mol	Joback Method
hvap	66.32	kJ/mol	Joback Method
log10ws	-7.56		Crippen Method
logp	6.070		Crippen Method
mcvol	257.010	ml/mol	McGowan Method
pc	1214.90	kPa	Joback Method
rinpol	1908.00		NIST Webbook
rinpol	1903.00		NIST Webbook
rinpol	1928.00		NIST Webbook
rinpol	1916.00		NIST Webbook
rinpol	1912.00		NIST Webbook
rinpol	1909.00		NIST Webbook
rinpol	1910.00		NIST Webbook
rinpol	1910.00		NIST Webbook
rinpol	1928.00		NIST Webbook
rinpol	1909.00		NIST Webbook
ripol	2199.00		NIST Webbook
ripol	2195.00		NIST Webbook
ripol	2185.00		NIST Webbook
ripol	2195.00		NIST Webbook
ripol	2195.00		NIST Webbook
ripol	2182.00		NIST Webbook
ripol	2185.00		NIST Webbook
ripol	2199.00		NIST Webbook
ripol	2185.00		NIST Webbook
tb	735.46	K	Joback Method

tc	908.12	K	Joback Method
tf	456.75	K	Joback Method
vc	1.050	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	747.94	J/mol×K	735.46	Joback Method
cpg	762.76	J/mol×K	764.24	Joback Method
cpg	776.83	J/mol×K	793.01	Joback Method
cpg	790.17	J/mol×K	821.79	Joback Method
cpg	802.80	J/mol×K	850.57	Joback Method
cpg	814.71	J/mol×K	879.35	Joback Method
cpg	825.91	J/mol×K	908.12	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373607&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

ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume