10-Chlorodecyl 2,3,4,5,6-pentafluorobenzoate

Inchi: InChI=1S/C17H20ClF5O2/c18-9-7-5-3-1-2-4-6-8-10-25-17(24)11-12(19)14(21)16(23)15(
InchiKey: ZKMAZQLQJOWAHS-UHFFFAOYSA-N
Formula: C17H20ClF5O2
SMILES: O=C(OCCCCCCCCCCCCl)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 386.79

Physical Properties

Property code	Value	Unit	Source
gf	-1063.38	kJ/mol	Joback Method
hf	-1456.12	kJ/mol	Joback Method
hfus	54.27	kJ/mol	Joback Method
hvap	68.48	kJ/mol	Joback Method
log10ws	-7.29		Crippen Method
logp	5.899		Crippen Method
mcvol	255.160	ml/mol	McGowan Method
pc	1266.45	kPa	Joback Method
rinpol	2124.00		NIST Webbook
rinpol	2124.00		NIST Webbook
tb	750.01	K	Joback Method
tc	926.79	K	Joback Method
tf	475.40	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.06	J/mol×K	750.01	Joback Method
cpg	734.62	J/mol×K	779.47	Joback Method
cpg	747.45	J/mol×K	808.94	Joback Method
cpg	759.57	J/mol×K	838.40	Joback Method
cpg	770.99	J/mol×K	867.86	Joback Method
cpg	781.71	J/mol×K	897.33	Joback Method
cpg	791.75	J/mol×K	926.79	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=U373591&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume