8-Chlorooctyl 2,3,4,5,6-pentafluorobenzoate

Inchi: InChI=1S/C15H16ClF5O2/c16-7-5-3-1-2-4-6-8-23-15(22)9-10(17)12(19)14(21)13(20)11(
InchiKey: YRUIEPYRCAHRFQ-UHFFFAOYSA-N
Formula: C15H16ClF5O2
SMILES: O=C(OCCCCCCCCCCl)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 358.73

Physical Properties

Property code	Value	Unit	Source
gf	-1080.22	kJ/mol	Joback Method
hf	-1414.84	kJ/mol	Joback Method
hfus	49.09	kJ/mol	Joback Method
hvap	64.03	kJ/mol	Joback Method
log10ws	-6.46		Crippen Method
logp	5.118		Crippen Method
mcvol	226.980	ml/mol	McGowan Method
pc	1459.02	kPa	Joback Method
rinpol	1925.00		NIST Webbook
rinpol	1937.00		NIST Webbook
tb	704.25	K	Joback Method
tc	878.93	K	Joback Method
tf	452.86	K	Joback Method
vc	0.930	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	612.20	J/mol×K	704.25	Joback Method
cpg	624.68	J/mol×K	733.36	Joback Method
cpg	636.54	J/mol×K	762.48	Joback Method
cpg	647.77	J/mol×K	791.59	Joback Method
cpg	658.39	J/mol×K	820.70	Joback Method
cpg	668.40	J/mol×K	849.82	Joback Method
cpg	677.81	J/mol×K	878.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373587&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

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