Pentafluorobenzoic acid, 3-chloroprop-2-enyl ester

Inchi: InChI=1S/C10H4ClF5O2/c11-2-1-3-18-10(17)4-5(12)7(14)9(16)8(15)6(4)13/h1-2H,3H2/b

InchiKey: LAYNCYUILTUINL-OWOJBTEDSA-N

Formula: C10H4ClF5O2

SMILES: O=C(OCC=CCl)c1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 286.58

Physical Properties

Property code	Value	Unit	Source
gf	-1042.10	kJ/mol	Joback Method
hf	-1194.42	kJ/mol	Joback Method
hfus	36.34	kJ/mol	Joback Method
hvap	52.85	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	3.291		Crippen Method
mcvol	152.230	ml/mol	McGowan Method
pc	2298.11	kPa	Joback Method
rinpol	1341.00		NIST Webbook
rinpol	1341.00		NIST Webbook
tb	594.01	K	Joback Method
tc	778.16	K	Joback Method
tf	391.43	K	Joback Method
vc	0.630	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.12	J/mol×K	594.01	Joback Method
cpg	351.48	J/mol×K	624.70	Joback Method
cpg	359.43	J/mol×K	655.39	Joback Method
cpg	366.97	J/mol×K	686.08	Joback Method
cpg	374.11	J/mol×K	716.78	Joback Method
cpg	380.86	J/mol×K	747.47	Joback Method
cpg	387.22	J/mol×K	778.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299191&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