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

Other names: Pentafluorobenzoic acid, 2,2,2-trichloroethyl ester
Inchi: InChI=1S/C9H2Cl3F5O2/c10-9(11,12)1-19-8(18)2-3(13)5(15)7(17)6(16)4(2)14/h1H2
InchiKey: YNOZJVPRCHEEIX-UHFFFAOYSA-N
Formula: C9H2Cl3F5O2
SMILES: O=C(OCC(Cl)(Cl)Cl)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 343.46
CAS: 84949-25-7

Physical Properties

Property code	Value	Unit	Source
gf	-1151.76	kJ/mol	Joback Method
hf	-1331.23	kJ/mol	Joback Method
hfus	34.53	kJ/mol	Joback Method
hvap	58.14	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	3.909		Crippen Method
mcvol	166.920	ml/mol	McGowan Method
pc	2274.07	kPa	Joback Method
rinpol	1447.00		NIST Webbook
rinpol	1441.00		NIST Webbook
rinpol	1441.00		NIST Webbook
tb	638.60	K	Joback Method
tc	835.61	K	Joback Method
tf	447.50	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	364.74	J/mol×K	638.60	Joback Method
cpg	371.92	J/mol×K	671.44	Joback Method
cpg	378.62	J/mol×K	704.27	Joback Method
cpg	384.85	J/mol×K	737.11	Joback Method
cpg	390.61	J/mol×K	769.94	Joback Method

cpg	395.92	J/mol×K	802.78	Joback Method
cpg	400.79	J/mol×K	835.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C84949257&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