Pentadecafluorooctanoic acid, 2,2-dichloroethyl ester

Inchi: InChI=1S/C10H3Cl2F15O2/c11-2(12)1-29-3(28)4(13,14)5(15,16)6(17,18)7(19,20)8(21,22

InchiKey: JRIWQWPDYOLSAY-UHFFFAOYSA-N

Formula: C10H3Cl2F15O2

SMILES: O=C(OCC(Cl)Cl)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 511.01

Physical Properties

Property code	Value	Unit	Source
gf	-3129.17	kJ/mol	Joback Method
hf	-3534.19	kJ/mol	Joback Method
hfus	23.62	kJ/mol	Joback Method
hvap	34.06	kJ/mol	Joback Method
log10ws	-6.33		Crippen Method
logp	5.707		Crippen Method
mcvol	210.230	ml/mol	McGowan Method
pc	1331.98	kPa	Joback Method
rinpol	1053.00		NIST Webbook
rinpol	1053.00		NIST Webbook
tb	545.35	K	Joback Method
tc	688.71	K	Joback Method
tf	345.25	K	Joback Method
vc	0.904	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.80	J/mol×K	545.35	Joback Method
cpg	584.44	J/mol×K	569.24	Joback Method
cpg	594.20	J/mol×K	593.14	Joback Method
cpg	603.13	J/mol×K	617.03	Joback Method
cpg	611.27	J/mol×K	640.92	Joback Method
cpg	618.69	J/mol×K	664.82	Joback Method
cpg	625.44	J/mol×K	688.71	Joback Method

Sources

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=U406807&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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