Succinic acid, 2-chlorophenyl 2,2,3,3,4,4,4-heptafluorobutyl ester

Inchi: InChI=1S/C14H10ClF7O4/c15-8-3-1-2-4-9(8)26-11(24)6-5-10(23)25-7-12(16,17)13(18,19

InchiKey: ROWRIQLLMZXVME-UHFFFAOYSA-N

Formula: C14H10ClF7O4

SMILES: O=C(CCC(=O)Oc1ccccc1Cl)OCC(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 410.67

Physical Properties

Property code	Value	Unit	Source
gf	-1665.14	kJ/mol	Joback Method
hf	-2011.59	kJ/mol	Joback Method
hfus	34.76	kJ/mol	Joback Method
hvap	62.79	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.402		Crippen Method
mcvol	223.870	ml/mol	McGowan Method
pc	1667.33	kPa	Joback Method
rinpol	1748.00		NIST Webbook
tb	726.59	K	Joback Method
tc	913.55	K	Joback Method
tf	472.11	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.57	J/mol×K	726.59	Joback Method
cpg	639.17	J/mol×K	757.75	Joback Method
cpg	648.93	J/mol×K	788.91	Joback Method
cpg	657.92	J/mol×K	820.07	Joback Method
cpg	666.18	J/mol×K	851.23	Joback Method
cpg	673.76	J/mol×K	882.39	Joback Method
cpg	680.73	J/mol×K	913.55	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=U357545&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