Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl 2,6-dichlorophenyl ester

Inchi: InChI=1S/C15H10Cl2F8O4/c16-7-2-1-3-8(17)11(7)29-10(27)5-4-9(26)28-6-13(20,21)15(2

InchiKey: IYSBFXZVGJRTSA-UHFFFAOYSA-N

Formula: C15H10Cl2F8O4

SMILES: O=C(CCC(=O)Oc1c(Cl)cccc1Cl)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 477.13

Physical Properties

Property code	Value	Unit	Source
gf	-1875.53	kJ/mol	Joback Method
hf	-2260.83	kJ/mol	Joback Method
hfus	40.71	kJ/mol	Joback Method
hvap	68.85	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	5.393		Crippen Method
mcvol	251.970	ml/mol	McGowan Method
pc	1441.35	kPa	Joback Method
rinpol	2038.00		NIST Webbook
rinpol	2038.00		NIST Webbook
tb	790.71	K	Joback Method
tc	980.64	K	Joback Method
tf	511.41	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.04	J/mol×K	790.71	Joback Method
cpg	720.69	J/mol×K	822.36	Joback Method
cpg	729.54	J/mol×K	854.02	Joback Method
cpg	737.66	J/mol×K	885.67	Joback Method
cpg	745.09	J/mol×K	917.33	Joback Method
cpg	751.89	J/mol×K	948.98	Joback Method
cpg	758.12	J/mol×K	980.64	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=U389864&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