Succinic acid, 4-chloro-3-methylphenyl 2,2,3,4,4,4-hexafluorobutyl ester

Inchi: InChI=1S/C15H13ClF6O4/c1-8-6-9(2-3-10(8)16)26-12(24)5-4-11(23)25-7-14(18,19)13(17

InchiKey: HKDGFIMGBVRJKT-UHFFFAOYSA-N

Formula: C15H13ClF6O4

SMILES: Cc1cc(OC(=O)CCC(=O)OCC(F)(F)C(F)C(F)(F)F)ccc1Cl

Mol. weight [g/mol]: 406.70

Physical Properties

Property code	Value	Unit	Source
gf	-1476.82	kJ/mol	Joback Method
hf	-1844.12	kJ/mol	Joback Method
hfus	37.77	kJ/mol	Joback Method
hvap	67.40	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	4.413		Crippen Method
mcvol	236.190	ml/mol	McGowan Method
pc	1567.23	kPa	Joback Method
rinpol	1975.00		NIST Webbook
rinpol	1975.00		NIST Webbook
tb	757.97	K	Joback Method
tc	946.87	K	Joback Method
tf	477.89	K	Joback Method
vc	0.945	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	670.35	J/mol×K	757.97	Joback Method
cpg	681.66	J/mol×K	789.45	Joback Method
cpg	692.14	J/mol×K	820.94	Joback Method
cpg	701.83	J/mol×K	852.42	Joback Method
cpg	710.76	J/mol×K	883.90	Joback Method
cpg	718.98	J/mol×K	915.39	Joback Method
cpg	726.51	J/mol×K	946.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390810&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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