Succinic acid, 2,2,3,3-tetrafluoropropyl (2-chlorocyclohexyl)methyl ester

Inchi: InChI=1S/C14H19ClF4O4/c15-10-4-2-1-3-9(10)7-22-11(20)5-6-12(21)23-8-14(18,19)13(1

InchiKey: LBHWWXBISSCPSI-UHFFFAOYSA-N

Formula: C14H19ClF4O4

SMILES: O=C(CCC(=O)OCC(F)(F)C(F)F)OCC1CCCCC1Cl

Mol. weight [g/mol]: 362.75

Physical Properties

Property code	Value	Unit	Source
gf	-1174.87	kJ/mol	Joback Method
hf	-1602.12	kJ/mol	Joback Method
hfus	36.08	kJ/mol	Joback Method
hvap	64.62	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.551		Crippen Method
mcvol	231.460	ml/mol	McGowan Method
pc	1615.47	kPa	Joback Method
rinpol	1967.00		NIST Webbook
rinpol	1967.00		NIST Webbook
tb	718.02	K	Joback Method
tc	905.66	K	Joback Method
tf	414.70	K	Joback Method
vc	0.903	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.05	J/mol×K	718.02	Joback Method
cpg	698.41	J/mol×K	749.29	Joback Method
cpg	712.76	J/mol×K	780.57	Joback Method
cpg	726.12	J/mol×K	811.84	Joback Method
cpg	738.53	J/mol×K	843.11	Joback Method
cpg	749.99	J/mol×K	874.39	Joback Method
cpg	760.52	J/mol×K	905.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391397&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