Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl (2-chlorocyclohexyl)methyl ester

Inchi: InChI=1S/C16H19ClF8O4/c17-10-4-2-1-3-9(10)7-28-11(26)5-6-12(27)29-8-14(20,21)16(2

InchiKey: GUSNVUYJRFYCQD-UHFFFAOYSA-N

Formula: C16H19ClF8O4

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

Mol. weight [g/mol]: 462.76

Physical Properties

Property code	Value	Unit	Source
gf	-1931.59	kJ/mol	Joback Method
hf	-2445.34	kJ/mol	Joback Method
hfus	38.75	kJ/mol	Joback Method
hvap	63.22	kJ/mol	Joback Method
log10ws	-5.42		Crippen Method
logp	4.822		Crippen Method
mcvol	266.720	ml/mol	McGowan Method
pc	1255.70	kPa	Joback Method
rinpol	2051.00		NIST Webbook
rinpol	2051.00		NIST Webbook
tb	754.40	K	Joback Method
tc	934.38	K	Joback Method
tf	444.44	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	829.94	J/mol×K	754.40	Joback Method
cpg	844.44	J/mol×K	784.40	Joback Method
cpg	857.92	J/mol×K	814.39	Joback Method
cpg	870.41	J/mol×K	844.39	Joback Method
cpg	881.97	J/mol×K	874.39	Joback Method
cpg	892.64	J/mol×K	904.39	Joback Method
cpg	902.48	J/mol×K	934.38	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391398&Units=SI

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