

Succinic acid, 1,1,1-trifluoroprop-2-yl 4-chloro-2-methylphenyl ester

Inchi:	InChI=1S/C14H14ClF3O4/c1-8-7-10(15)3-4-11(8)22-13(20)6-5-12(19)21-9(2)14(16,17)18
InchiKey:	ZALHTXUTIKYBAC-UHFFFAOYSA-N
Formula:	C14H14ClF3O4
SMILES:	Cc1cc(Cl)ccc1OC(=O)CCC(=O)OC(C)C(F)(F)F
Mol. weight [g/mol]:	338.71

Physical Properties

Property code	Value	Unit	Source
gf	-903.65	kJ/mol	Joback Method
hf	-1226.40	kJ/mol	Joback Method
hfus	33.35	kJ/mol	Joback Method
hvap	68.92	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	3.828		Crippen Method
mcvol	216.790	ml/mol	McGowan Method
pc	1867.55	kPa	Joback Method
rinpola	1801.00		NIST Webbook
rinpola	1801.00		NIST Webbook
tb	740.51	K	Joback Method
tc	940.87	K	Joback Method
tf	462.43	K	Joback Method
vc	0.846	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.27	J/mol×K	740.51	Joback Method
cpg	603.34	J/mol×K	773.90	Joback Method
cpg	614.55	J/mol×K	807.30	Joback Method
cpg	624.92	J/mol×K	840.69	Joback Method
cpg	634.47	J/mol×K	874.08	Joback Method
cpg	643.22	J/mol×K	907.47	Joback Method
cpg	651.21	J/mol×K	940.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390285&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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