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

Inchi: InChI=1S/C14H14ClF3O5/c1-8(14(16,17)18)22-12(19)5-6-13(20)23-10-4-3-9(15)7-11(10

InchiKey: SRZMQMCTONTFDI-UHFFFAOYSA-N

Formula: C14H14ClF3O5

SMILES: COc1cc(Cl)ccc1OC(=O)CCC(=O)OC(C)C(F)(F)F

Mol. weight [g/mol]: 354.71

Physical Properties

Property code	Value	Unit	Source
gf	-1008.65	kJ/mol	Joback Method
hf	-1358.62	kJ/mol	Joback Method
hfus	34.54	kJ/mol	Joback Method
hvap	71.33	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.528		Crippen Method
mcvol	222.660	ml/mol	McGowan Method
pc	1840.41	kPa	Joback Method
rinpol	1943.00		NIST Webbook
rinpol	1943.00		NIST Webbook
tb	762.93	K	Joback Method
tc	962.61	K	Joback Method
tf	484.66	K	Joback Method
vc	0.864	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.03	J/mol×K	762.93	Joback Method
cpg	628.81	J/mol×K	796.21	Joback Method
cpg	639.71	J/mol×K	829.49	Joback Method
cpg	649.73	J/mol×K	862.77	Joback Method
cpg	658.88	J/mol×K	896.05	Joback Method
cpg	667.18	J/mol×K	929.33	Joback Method
cpg	674.64	J/mol×K	962.61	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=U390928&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

Latest version available from:
https://www.chemeo.com/cid/121-435-4/Succinic-acid-1-1-1-trifluoroprop-2-yl-4-chloro-2-methoxyphenyl-ester.pdf
Generated by Cheméo on 2024-05-01 09:13:58.778637509 +0000 UTC m=+16844087.699214830.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.