

Succinic acid, 2,2,3,3-tetrafluoropropyl 1-cyclopentylethyl ester

Inchi:	InChI=1S/C14H20F4O4/c1-9(10-4-2-3-5-10)22-12(20)7-6-11(19)21-8-14(17,18)13(15)16
InchiKey:	FJGLZRSBFSMVDW-UHFFFAOYSA-N
Formula:	C14H20F4O4
SMILES:	CC(OC(=O)CCC(=O)OCC(F)(F)C(F)F)C1CCCC1
Mol. weight [g/mol]:	328.30

Physical Properties

Property code	Value	Unit	Source
gf	-1145.57	kJ/mol	Joback Method
hf	-1565.16	kJ/mol	Joback Method
hfus	29.39	kJ/mol	Joback Method
hvap	59.99	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.332		Crippen Method
mcvol	219.220	ml/mol	McGowan Method
pc	1686.56	kPa	Joback Method
rinpol	1685.00		NIST Webbook
rinpol	1685.00		NIST Webbook
tb	680.55	K	Joback Method
tc	862.27	K	Joback Method
tf	377.54	K	Joback Method
vc	0.858	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	648.02	J/molxK	680.55	Joback Method
cpg	663.74	J/molxK	710.84	Joback Method
cpg	678.52	J/molxK	741.12	Joback Method
cpg	692.40	J/molxK	771.41	Joback Method
cpg	705.41	J/molxK	801.70	Joback Method
cpg	717.56	J/molxK	831.99	Joback Method
cpg	728.89	J/molxK	862.27	Joback Method

Sources

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=U391407&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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